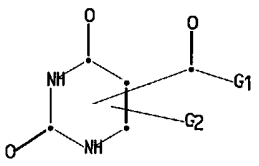
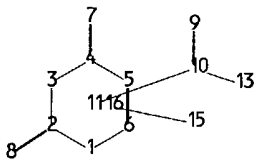
C:\Program Files\Common Files\System\Mapi\1033\NT





chain nodes :
7 8 9 10 13 15
ring nodes :
1 2 3 4 5 6
chain bonds :
2-8 4-7 9-10 10-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 4-5 4-7 5-6 9-10 10-13
isolated ring systems :
containing 1 :

G1:O,S,N,SO2

G2:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 15:CLASS 16:CLASS

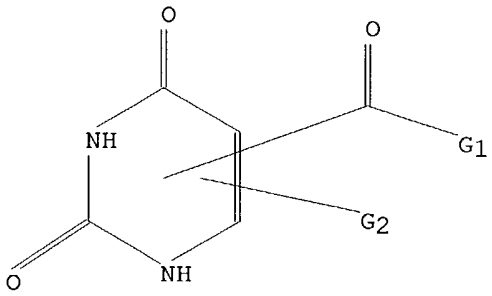
=> ....Testing the current file.... screen

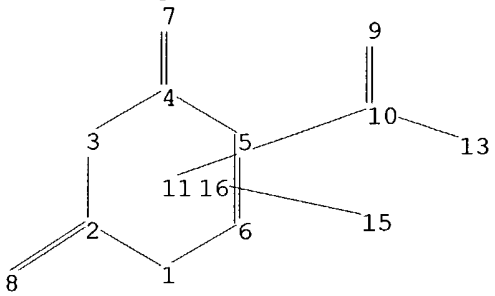
ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L1 SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10008277.str





chain nodes :
7 8 9 10 13 15
ring nodes :
1 2 3 4 5 6
chain bonds :
2-8 4-7 9-10 10-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 4-5 4-7 5-6 9-10 10-13
isolated ring systems :
containing 1 :

G1:O,S,N,SO2

G2:O,N

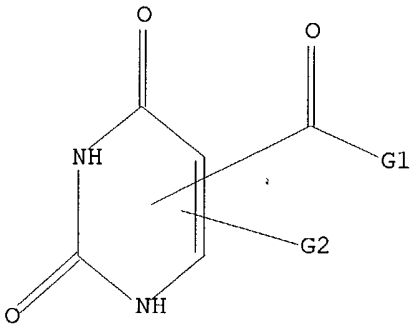
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 15:CLASS 16:CLASS

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

L3 QUE L2 NOT L1

=> d l3
L3 HAS NO ANSWERS
L1 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L2 STR



G1 O,S,N,SO2

G2 O,N

Structure attributes must be viewed using STN Express query preparation.
L3 QUE L2 NOT L1

=> s l3 sss sam
SAMPLE SEARCH INITIATED 17:38:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3935 TO ITERATE

25.4% PROCESSED 1000 ITERATIONS 11 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 74939 TO 82461
PROJECTED ANSWERS: 471 TO 1259

L4 11 SEA SSS SAM L2 NOT L1

=> => s l3 sss ful
FULL SEARCH INITIATED 17:43:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 80419 TO ITERATE

100.0% PROCESSED 80419 ITERATIONS 346 ANSWERS
SEARCH TIME: 00.00.01

L5 346 SEA SSS FUL L2 NOT L1

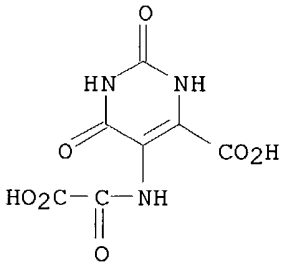
=> => s l5
L6 140 L5

=> d l6 1-50 bib,ab,hitstr

L6 ANSWER 1 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:45434 CAPLUS
DN 140:217289
TI Solid-phase synthesis of an oxalic acid amide library
AU Georgiadis, Taxiarchis M.; Baindur, Nand; Player, Mark R.
CS 3-Dimensional Pharmaceuticals Inc., Cranbury, NJ, 08512, USA
SO Journal of Combinatorial Chemistry (2004), 6(2), 224-229
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
AB Monoamides of oxalic acid are of interest as bioisosteric replacements for phosphate groups in the design of enzyme inhibitors. The use of oxalic acid as a linker to the Wang resin in the synthesis of individual or libraries of phosphate biosteres is demonstrated. The highly reactive resin-bound acid chloride reacts with arylamines to yield resin-bound N-aryloxamic acids (oxanilic acids). This methodol. is especially useful for the rapid synthesis of 2-(oxalylamino)benzoic acids, because it can be utilized for library synthesis and eliminates the intermediate purification step necessary in solution-phase reactions. The products are cleaved off the resin with trifluoroacetic acid in dichloromethane in good yields.

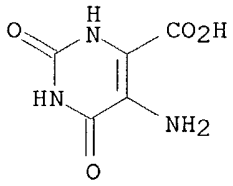
IT **243989-99-3P**
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(preparation of oxalic acid amides via solid-phase amidation of Wang resin-bound oxalyl chloride with aromatic amines)

RN 243989-99-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(carboxycarbonyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **7164-43-4**
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)
(preparation of oxalic acid amides via solid-phase amidation of Wang resin-bound oxalyl chloride with aromatic amines)

RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



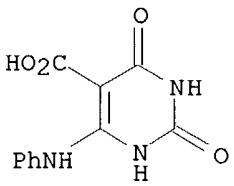
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:571128 CAPLUS
DN 139:129926
TI Crystal structures of human JNK3 kinase-inhibitor complexes and JNK3 active- and inhibitor-binding sites and applications to drug screening and drug design
IN Xie, Xiaoling
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 244 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003060102	A2	20030724	WO 2003-US899	20030110
WO 2003060102	A3	20031127		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

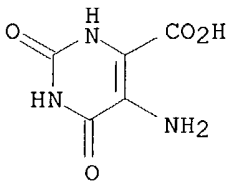
PRAI US 2002-348002P P 20020111
AB The invention relates to crystalline mols. or mol. complexes that comprise binding pockets of c-Jun N-terminal kinase 3 (JNK3) or its homologs. The invention also relates to crystals comprising JNK3 and an inhibitor. Crystal structure and atomic structure coordinates of human JNK3α1 complexes with various inhibitors are provided. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of JNK3 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the mol. or mol. complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compds., including agonists and antagonists, which bind to JNK3 or homologs thereof.
IT **565197-20-8D**, JNK3 complexes
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(crystal structures of JNK3 kinase-inhibitor complexes and JNK3 active- and inhibitor-binding sites and applications to drug screening and drug design)
RN 565197-20-8 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-2,4-dioxo-6-(phenylamino)- (9CI) (CA INDEX NAME)


O
HO2C
NH
PhNH
N
H
O

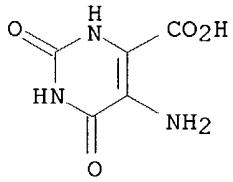
L6 ANSWER 3 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:814111 CAPLUS
DN 137:325426
TI Preparation of pyrimidine derivatives as anti-ictogenic and/or anti-epileptogenic agents
IN Weaver, Donald F.; Guillain, Buhendwa Musole; Carran, John R.; Jones, Kathryn
PA Queen's University At Kingston, Can.
SO PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002083651	A2	20021024	WO 2002-CA512	20020411
	WO 2002083651	A3	20021219		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003153584	A1	20030814	US 2002-123062	20020411
	EP 1385831	A2	20040204	EP 2002-717913	20020411
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2003194375	A1	20031016	US 2002-272249	20021015
PRAI	US 2001-282987P	P	20010411		
	US 2001-285940P	P	20010423		
	US 2001-310748P	P	20010807		
	US 2002-99934	A	20020313		
	US 2001-275618P	P	20010313		
	WO 2002-CA512	W	20020411		

OS MARPAT 137:325426
AB Title compds., e.g., I [R9 = H, alkyl, alkynyl, aryl, amino, etc.; R10 = H, alkyl, aryl, carboxyl, etc.; R11 = H, alkyl, amino, thioether, tetrahydrofuranyl] and derivs. thereof were prepared For instance, 5-hydroxymethyuracil (II) was prepared from uracil and formaldehyde (KOHaq, 50°, 72 h). II and other example compds. tested were active in the hippocampal kindling seizure model. I are useful for the inhibition of convulsive disorders including epilepsy.
IT **7164-43-4P**, 5-Amino-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine (uracil) derivs. as antiepileptic agents)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:549402 CAPLUS
DN 138:85325
TI The Cold Origin of Life: B. Implications Based on Pyrimidines and Purines Produced From Frozen Ammonium Cyanide Solutions
AU Miyakawa, Shin; Cleaves, H. James; Miller, Stanley L.
CS Faculty of Engineering, Department of Chemistry and Biotechnology, Yokohama National University, Yokohama, 240-8501, Japan
SO Origins of Life and Evolution of the Biosphere (2002), 32(3), 209-218
CODEN: OLEBEM; ISSN: 0169-6149
PB Kluwer Academic Publishers
DT Journal
LA English
AB A wide variety of pyrimidines and purines were identified as products of a dilute frozen ammonium cyanide solution that had been held at -78° for 27 yr. This demonstrates that both pyrimidines and purines could have been produced on the primitive earth in a short time by eutectic concentration of HCN, even though the concentration of HCN in the primitive ocean may have been low. We suggest that eutectic freezing is the most plausible demonstrated mechanism by which HCN polymns. could have produced biol. important prebiotic compds.
IT **7164-43-4P**, 5-AminoOrotic acid
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(pyrimidines and purines produced from frozen ammonium cyanide solns. and origin of life)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:487577 CAPLUS
DN 137:63420
TI Preparation of lactone ketolide macrolide erythromycin antibiotics
IN Andreotti, Daniele; Arista, Luca; Biondi, Stefano; Cardullo, Francesca; Damiani, Frederica; Lociuro, Sergio; Marchioro, Carla; Merlo, Giancarlo; Mingardi, Anna; Niccolai, Daniela; Paio, Alfredo; Piga, Elisabetta; Pozzan, Alfonso; Seri, Catia; Tarsi, Luca; Terreni, Silvia; Tibasco, Jessica
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 215 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

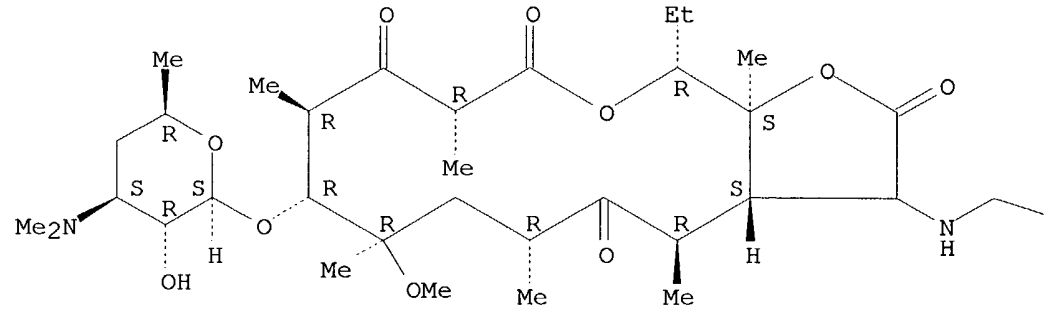
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002050091	A1	20020627	WO 2001-GB5665	20011220
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002017277	A5	20020701	AU 2002-17277	20011220
	EP 1363925	A1	20031126	EP 2001-271380	20011220
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	NO 2003002846	A	20030820	NO 2003-2846	20030620
	US 2004077557	A1	20040422	US 2003-450893	20031119
PRAI	GB 2000-31309	A	20001221		
	GB 2001-26276	A	20011101		
	GB 2001-26277	A	20011101		
	WO 2001-GB5665	W	20011220		

OS MARPAT 137:63420
AB The present invention relates to lactone ketolides I wherein R is H, CN, substituted alkyl; R1 is alkyl, alkenyl; R2 is H, hydroxy protecting group; R3 is H, halogen, and pharmaceutically acceptable salts and solvates thereof, to process for their preparation and their use in therapy or prophylaxis of systemic or topical bacterial infections in a human or animal body. Thus, (11S,21R)-3-decladinosyl-11,12-dideoxy-6-O-methyl-3-oxo-12,11-[oxycarbonyl-(cyano)-methylene]erythromycin A was prepared and tested as antibacterial agent against Streptococcus pneumoniae and Streptococcus pyogenes (MIC ≤ 1 μg/mL).
IT **439105-43-8P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)
RN 439105-43-8 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-amino-N-[2-[[(3aS,4R,6R,8R,9R,10R,12R,15R,15aS)-15-ethyltetradecahydro-8-methoxy-4,6,8,10,12,15a-hexamethyl-2,5,11,13-tetraoxo-9-[[3,4,6-trideoxy-3-(dimethylamino)-β-D-xylo-

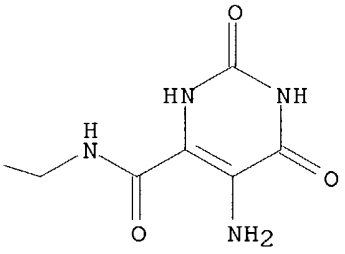
hexopyranosyl]oxy]-2H-furo[2,3-c]oxacyclotetradecin-3-yl]amino]ethyl]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

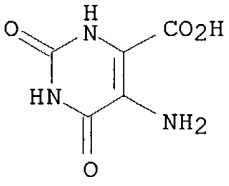
PAGE 1-A



PAGE 1-B

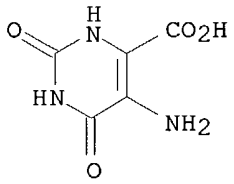


IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:71100 CAPLUS
DN 136:355098
TI Controlled stepwise conversion of 2,4,6,8-tetrachloropyrimido[5,4-d]pyrimidine into 2,4,6,8-tetrasubstituted pyrimido[5,4-d]pyrimidines
AU Northen, Julian S.; Boyle, F. Thomas; Clegg, William; Curtin, Nicola J.; Edwards, Andrew J.; Griffin, Roger J.; Golding, Bernard T.
CS Department of Chemistry, University of Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SO Journal of the Chemical Society, Perkin Transactions 1 (2002), (1), 108-115
CODEN: JCSPCE; ISSN: 1472-7781
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 136:355098
AB For the rational synthesis of 2,4,6,8-tetrasubstituted pyrimido[5,4-d]pyrimidines, required as purine mimetics, sequential nucleophilic substitutions of 2,4,6,8-tetrachloropyrimido[5,4-d]pyrimidine have been investigated. Reaction conditions have been devised leading to 2,4,6,8-tetrasubstituted pyrimido[5,4-d]pyrimidines, e.g. I, with patterns of substitution denoted as abab (reaction with nucleophile 1 at C-4 and C-8, followed by nucleophile 2 at C-2 and C-6) or abac (reaction with nucleophile 1 at C-4 and C-8, nucleophile 2 at C-2 and nucleophile 3 at C-6) or abcd (reaction with nucleophile 1 at C-4, nucleophile 2 at C-8, nucleophile 3 at C-2 and nucleophile 4 at C-6). The use of low temperature, relatively dilute solution and careful addition of the amine nucleophile can control the critical first step. The third step in the production of the abcd pattern leads to two regioisomers, which have been structurally characterized by 1H NMR and a crystal structure anal. Selected 2,4,6,8-tetrasubstituted pyrimido[5,4-d]pyrimidines were tested as inhibitors of the cyclin-dependent kinase complex (cyclin B/CDK1), but none of the compds. showed significant activity.
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(controlled stepwise conversion of 2,4,6,8-tetrachloropyrimido[5,4-d]pyrimidine into 2,4,6,8-tetrasubstituted pyrimido[5,4-d]pyrimidines)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



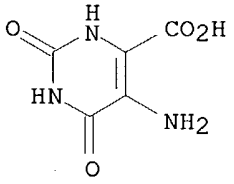
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:569519 CAPLUS
DN 135:156710
TI Method for prevention of corrosion of steel reinforcing bar in concrete
IN Nakayama, Norio
PA Ministry of Economy, Trade and Industry; National Industrial Research Institute, Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001213649	A2	20010807	JP 2000-20319	20000128
	JP 3289067	B2	20020604		
PRAI	JP 2000-20319		20000128		

AB A heterocyclic compound, which contains 5- or 6-membered ring comprising plural N and C atoms where ≥1 of C atoms are resonated with adjoining N atoms to form carbonyl group or its derivs., is mixed with a cement mixture, and it is used for producing concrete, mortar, or cement paste for preventing steel reinforcing bars in it from corrosion. The heterocyclic compound may be dissolved in H2O or organic solvents, and the resulting solution is applied on, sprayed to, or injected into the existing concrete, mortar, or cement paste structures for corrosion prevention of reinforcing bars in them. Corrosion of reinforcing bars can be easily prevented for a long period.

IT **7164-43-4**, 5-Aminoorotic acid
RL: TEM (Technical or engineered material use); USES (Uses)
(prevention of corrosion of steel reinforcing bar in concrete by using cyclic ureido derivative as corrosion inhibitor)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 8 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:319864 CAPLUS
DN 134:340357
TI Novel compounds, specifically aromatic and heteroaromatic ureas and thioureas, useful against parasites and especially against coccidiosis.
IN Muzi, Sabrina; Abdul-Rahman, Shoaa
PA New Pharma Research Sweden AB, Swed.
SO PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001030749	A1	20010503	WO 2000-SE2091	20001027
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1224165	A1	20020724	EP 2000-973336	20001027
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	EP 1210950	A1	20020605	EP 2000-850205	20001204
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	WO 2002045751	A1	20020613	WO 2001-SE2654	20011130
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002024308	A5	20020618	AU 2002-24308	20011130
PRAI	SE 1999-3894	A	19991028		
	WO 2000-SE2091	W	20001027		
	EP 2000-850205	A	20001204		
	WO 2001-SE2654	W	20011130		

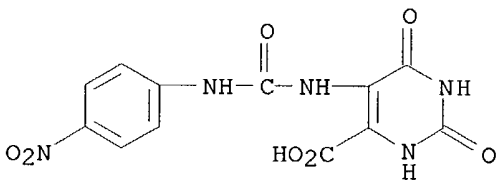
OS MARPAT 134:340357
AB The invention relates to novel ureas and thioureas R-C(:Y)-R [I; Y = O or S; R's are selected from the pairings: (a) NHR1 and NHR2, or (b) NR3R4 and NR5R6, or (c) NR3R4 and cyclic radical -N:Z-R7; R1, R2 = certain (un)substituted aryl, aralkyl, alkyl, heteroaryl, etc.; R3-R6 = certain (un)substituted aryl, aralkyl, or alkyl groups; Z = atoms to form ring; R7 = electron-withdrawing substituent] and their tautomers, solvates, radiolabeled derivs., and pharmaceutically acceptable salts. Also disclosed are pharmaceutical compns. containing I, as well as a method for treatment of parasitic disorders using I. I are especially well-suited for treatment of coccidiosis, particularly in poultry. Over 200 compds. are

listed, and several synthetic examples are given. For instance, reaction of PhNCS with 4-amino-3,5-diiodobenzoic acid in refluxing acetone in the presence of aqueous 10% KOH gave 75% thiourea derivative II. This compound had an anticoccidial effect in chickens similar to coxistac, but with a shorter duration of infection, reduced feed consumption, and no loss of growth rate.

IT **337531-83-6P**, 5-[[(4-Nitroanilino)carbonyl]amino]-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(parasiticide candidate; preparation of aromatic and heteroarom. ureas and thioureas as antiparasitic and anticoccidial agents)

RN 337531-83-6 CAPLUS

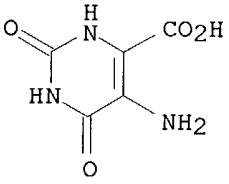
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[[[(4-nitrophenyl)amino]carbonyl]amino]-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **7164-43-4**, 5-Amino-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; preparation of aromatic and heteroarom. ureas and thioureas as antiparasitic and anticoccidial agents)

RN 7164-43-4 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

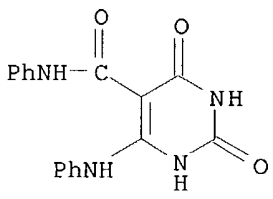


RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

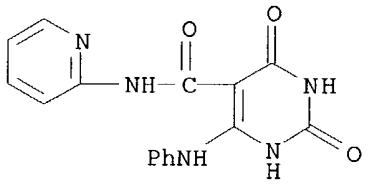
L6 ANSWER 9 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:881129 CAPLUS
DN 134:42135
TI Preparation of pyrimidinediones as inhibitors of c-JUN N-terminal kinases.
IN Salituro, Francesco; Bemis, Guy; Green, Jeremy; Fejzo, Jasna; Xie, Xiaoling
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000075118	A1	20001214	WO 2000-US15248	20000602
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2003100549	A1	20030529	US 2001-8277	20011203
PRAI	US 1999-137523P	P	19990603		
	WO 2000-US15248	A1	20000602		

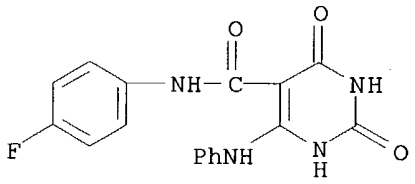
OS MARPAT 134:42135
AB Title compds. [I; Y = O, NH, NR, S, SO, SO2; X = O, NH, NR; R1, R2 = H, (substituted) alkyl, alkenyl, (aromatic) (bicyclic) carbocyclyl, heterocyclyl; R = alkyl, alkenyl, (aromatic) (bicyclic) carbocyclyl, heterocyclyl], were prepared as inhibitors of c-JUN N-terminal kinases. Thus, I (R1Y, R2X = PhNH) inhibited JNK3 with IC50 <1 μM.
IT **264884-33-5 312752-09-3 312752-10-6**
312752-12-8 312752-13-9 312752-15-1
312752-17-3 312752-19-5 312752-21-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of pyrimidinediones as inhibitors of c-JUN N-terminal kinases)
RN 264884-33-5 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-2,4-dioxo-N-phenyl-6-(phenylamino)- (9CI) (CA INDEX NAME)



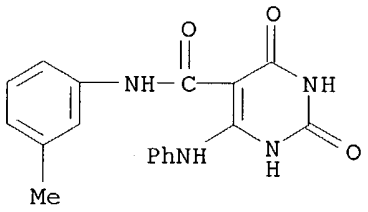
RN 312752-09-3 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-2,4-dioxo-6-(phenylamino)-N-2-pyridinyl- (9CI) (CA INDEX NAME)



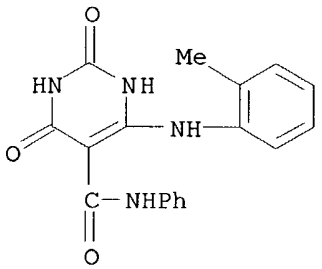
RN 312752-10-6 CAPLUS
CN 5-Pyrimidinecarboxamide, N-(4-fluorophenyl)-1,2,3,4-tetrahydro-2,4-dioxo-6-(phenylamino)- (9CI) (CA INDEX NAME)



RN 312752-12-8 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-N-(3-methylphenyl)-2,4-dioxo-6-(phenylamino)- (9CI) (CA INDEX NAME)

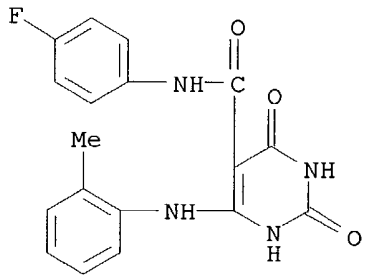


RN 312752-13-9 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-6-[(2-methylphenyl)amino]-2,4-dioxo-N-phenyl- (9CI) (CA INDEX NAME)

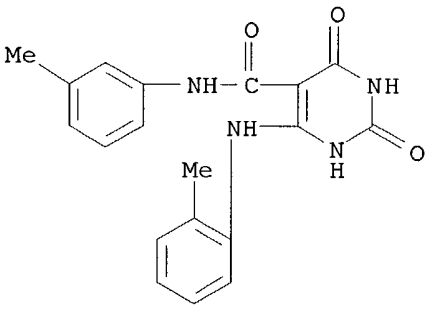


RN 312752-15-1 CAPLUS
CN 5-Pyrimidinecarboxamide, N-(4-fluorophenyl)-1,2,3,4-tetrahydro-6-[(2-

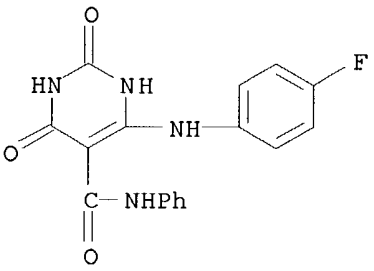
methylphenyl)amino]-2,4-dioxo- (9CI) (CA INDEX NAME)



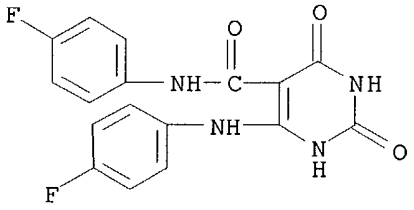
RN 312752-17-3 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-N-(3-methylphenyl)-6-[(2-methylphenyl)amino]-2,4-dioxo- (9CI) (CA INDEX NAME)



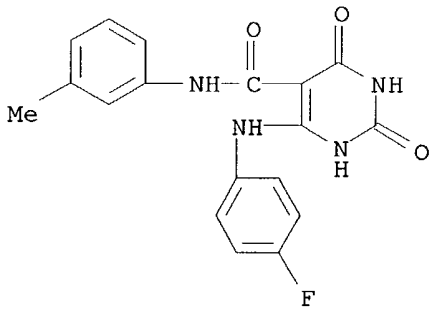
RN 312752-19-5 CAPLUS
CN 5-Pyrimidinecarboxamide, 6-[(4-fluorophenyl)amino]-1,2,3,4-tetrahydro-2,4-dioxo-N-phenyl- (9CI) (CA INDEX NAME)



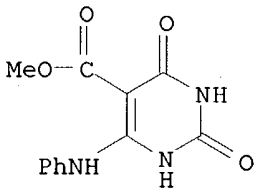
RN 312752-21-9 CAPLUS
CN 5-Pyrimidinecarboxamide, N-(4-fluorophenyl)-6-[(4-fluorophenyl)amino]-1,2,3,4-tetrahydro-2,4-dioxo- (9CI) (CA INDEX NAME)



IT **312752-23-1P 312752-25-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinediones as inhibitors of c-JUN N-terminal kinases)
RN 312752-23-1 CAPLUS
CN 5-Pyrimidinecarboxamide, 6-[(4-fluorophenyl)amino]-1,2,3,4-tetrahydro-N-(3-methylphenyl)-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 312752-25-3 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-2,4-dioxo-6-(phenylamino)-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:725485 CAPLUS
DN 133:296658
TI Preparation of desleucyl glycopeptide antibiotics
IN Kahne, Daniel; Walker, Suzanne; Silva, Domingos J.
PA The Trustees of Princeton University, USA; Incara Pharmaceuticals, Inc.
SO PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000059528	A1	20001012	WO 2000-US8559	20000331
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1173193	A1	20020123	EP 2000-919942	20000331
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	US 6518243	B1	20030211	US 2000-540761	20000331
PRAI	US 1999-127516P	P	19990402		
	WO 2000-US8559	W	20000331		

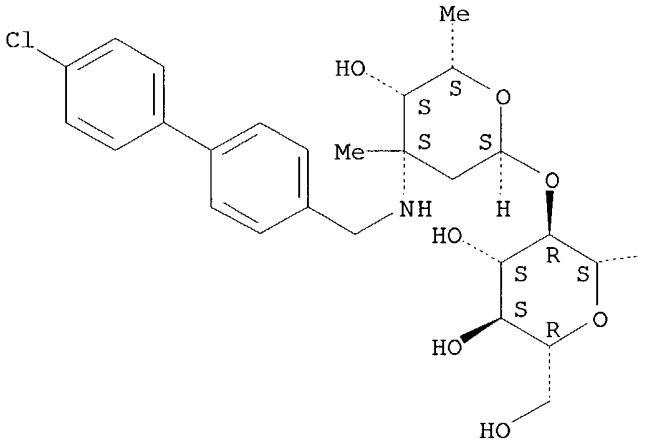
AB Compds. that are analogs of glycopeptide antibiotics are disclosed. The compds. have the formula A1-A2-A3-A4-A5-A6-A7, where each of the groups A2 to A7 is a modified or unmodified α-amino acid residue, A1 is optional and, when present, is an organic group other than N-substituted leucine, and at least one of the groups A1 to A7 is linked via a glycosidic bond to one or more glycosidic groups each having one or more sugar residues, where at least one of said sugar residues is modified to bear at least one hydrophobic substituent. Methods of making these compds., compns. including these compds., and methods of using the compds. to treat infections in a host are also disclosed. Antibacterial test data are tabulated for > 350 compds. of the invention.

IT **300580-49-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of desleucyl glycopeptide antibiotics)

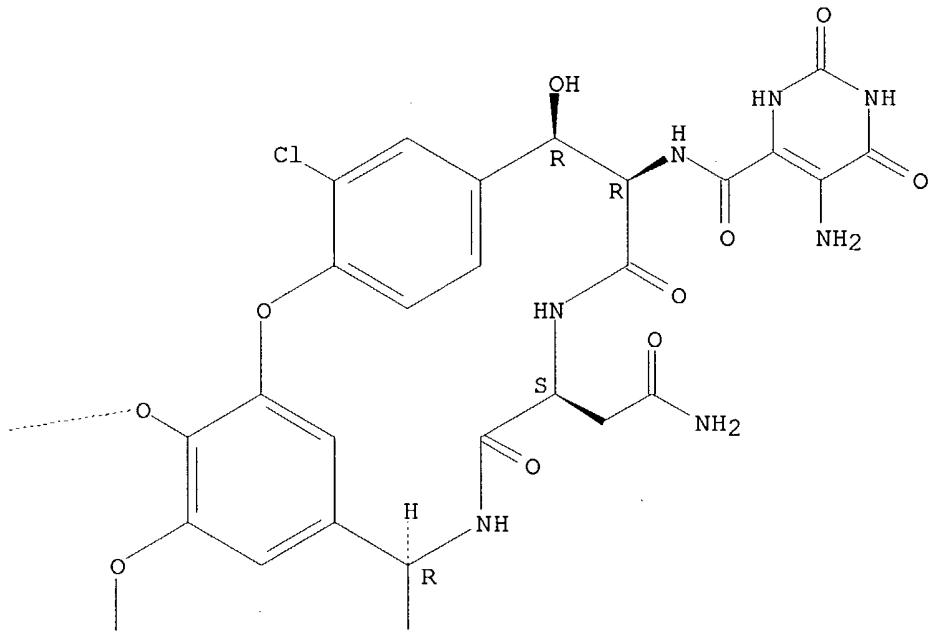
RN 300580-49-8 CAPLUS
CN Vancomycin, 49-[(5-amino-1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinyl)carbonyl]-N3''-[(4'-chloro[1,1'-biphenyl]-4-yl)methyl]-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



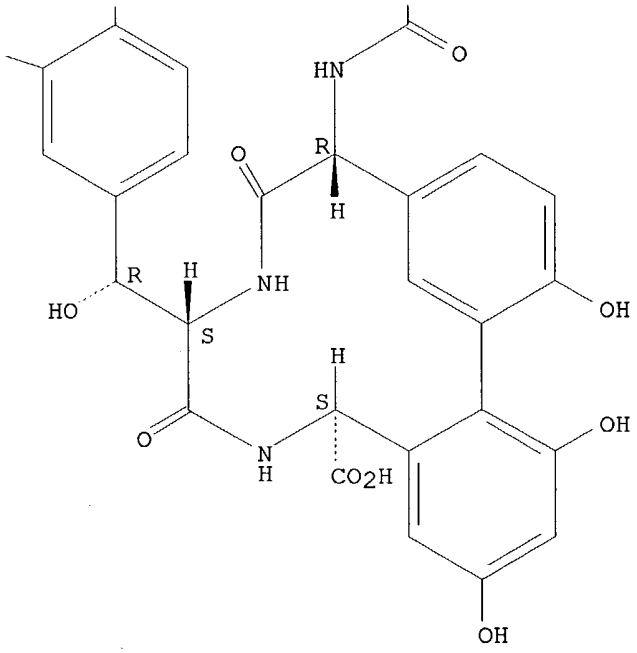
PAGE 1-B



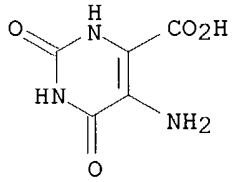
PAGE 2-A

Cl

PAGE 2-B

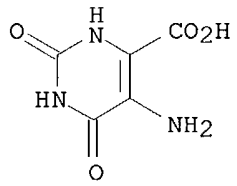


IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of desleucyl glycopeptide antibiotics)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

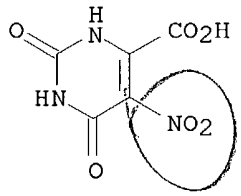


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:459129 CAPLUS
DN 133:189652
TI Catalytic properties of dihydroorotate dehydrogenase from Saccharomyces cerevisiae: studies on pH, alternate substrates, and inhibitors
AU Jordan, Douglas B.; Bisaha, John J.; Picollelli, Michael A.
CS Experimental Station, DuPont Pharmaceutical Company, Wilmington, DE, 19880-0400, USA
SO Archives of Biochemistry and Biophysics (2000), 378(1), 84-92
CODEN: ABBIA4; ISSN: 0003-9861
PB Academic Press
DT Journal
LA English
AB Yeast dihydroorotate dehydrogenase (DHOD) was purified 2800-fold to homogeneity from its natural source. Its sequence is 70% identical to that of the Lactococcus lactis DHOD (family IA) and the two active sites are nearly the same. Incubations of the yeast DHOD with dideuterodihydroorotate (deuterated in the positions eliminated in the dehydrogenation) as the donor and [14C]orotate as the acceptor revealed that the C5 deuteron exchanged with H2O solvent at a rate equal to the 14C exchange rate, whereas the C6 deuteron was infrequently exchanged with H2O solvent, thus indicating that the C6 deuteron of the dihydroorotate is sticky on the flavin cofactor. The pH dependencies of the steady-state parameters (kcat and kcat/Km) are similar, indicating that kcat/Km reports the productive binding of substrate, and the parameters are dependent on the donor-acceptor pair. The lower pKa values for kcat and kcat/Km observed for substrate dihydroorotate (around 6) in comparison to the values determined for dihydrooxonate (around 8) suggest that the C5 pro S hydrogen atom of dihydroorotate (but not the analogous hydrogen of dihydrooxonate), which is removed in the dehydrogenation, assists in lowering the pKa of the active site base (Cys133). The pH dependencies of the kinetic isotope effects on steady-state parameters observed for the dideuterated dihydroorotate are consistent with the dehydrogenation of substrate being rate limiting at low pH values, with a pKa value approximating that assigned to Cys133. Electron acceptors with dihydroorotate as donor were preferred in the following order: ferricyanide (1), DCPIP (0.54), Q0 (0.28), fumarate (0.15), and O2 (0.035). Orotate inhibition profiles vs. varied concns. of dihydroorotate with ferricyanide or O2 as acceptors suggest that both orotate and dihydroorotate have significant affinities for the reduced and oxidized forms of the enzyme. (c) 2000 Academic Press.
IT **7164-43-4**, 5-Aminoorotic acid **17687-24-0**, 5-Nitroorotic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition; catalytic properties of dihydroorotate dehydrogenase from Saccharomyces cerevisiae examined by studies on pH, alternate substrates, and inhibitors)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



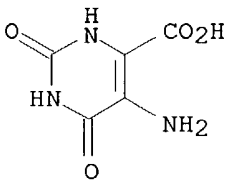
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:428138 CAPLUS
DN 133:77396
TI Heterocyclic inhibitor for preventing macrocell corrosion of steel encapsulated in concrete or mortar
IN Nakayama, Norio
PA Agency of Industrial Sciences and Technology, Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

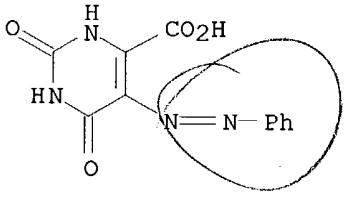
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2000178772	A2	20000627	JP 1998-356575	19981215
	JP 3018182	B2	20000313		
PRAI	JP 1998-356575		19981215		

AB A corrosion inhibitor consists of a heterocyclic compound having a 5- or 7-membered ring containing ≥2 N atoms and C atoms forming ≥1 carbonyl group adjacent to the N atoms, or of a derivative of such a compound Preferably the corrosion inhibitor is an aqueous solution of uramil, uramildiacetic acid, violuric acid, 4-aminourasil, 5-aminourasil, uric acid, 5-aminoorotic acid, their derivs., or salts. The inhibitor is coated on the outer surface of concrete, cement mortar, or cement paste basic structures formed around metal material such as tubes or reinforcing members to prevent macrocell corrosion.

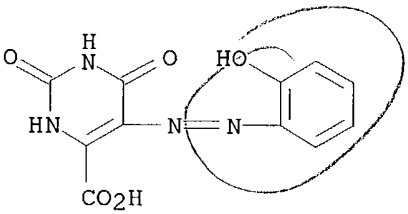
IT **7164-43-4**, 5-Aminoorotic acid
RL: TEM (Technical or engineered material use); USES (Uses)
(heterocyclic inhibitor for preventing macrocell corrosion of steel encapsulated in concrete or cement mortar)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



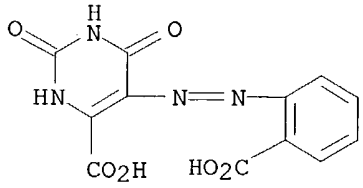
L6 ANSWER 13 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:163599 CAPLUS
DN 132:329018
TI Synthesis and structural chemistry of iron complexes containing arylazo orotic acid
AU El-Marghany, A.
CS Chemistry Department, Suez Canal University, Suez, Egypt
SO Mansoura Science Bulletin, A: Chemistry (1999), 26(2), 47-55
CODEN: MSBCF4; ISSN: 1110-4562
PB Mansoura University
DT Journal
LA English
AB Arylazo orotic acid complexes of Fe(III) were prepared, and identified by elemental anal., IR, UV-visible spectral and the magnetic susceptibility values. The complexes are with Oh geometry. The Mossbauer spectra of Fe complexes derived from orotic acid (O.A.) and its o-OH and o-COOH arylazo O.A. are measured and discussed. The isomer shift values for the complexes are less than the high spin FeIII complexes (δ = 0.5-0.7 mm/s), probably due to the increase in the electron d. at the nucleus.
IT **155984-14-8 155984-17-1 155984-18-2 155984-19-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of iron(III) arylazo orotic acid complex)
RN 155984-14-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-(phenylazo)-(9CI) (CA INDEX NAME)



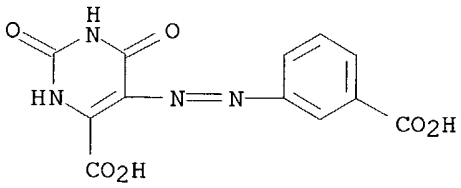
RN 155984-17-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(2-hydroxyphenyl)azo]-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 155984-18-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(2-carboxyphenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 155984-19-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-carboxyphenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

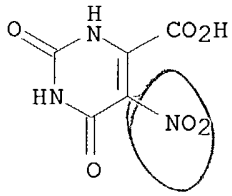


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

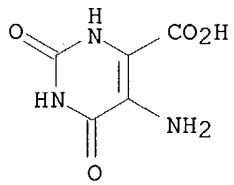
L6 ANSWER 14 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:15701 CAPLUS
DN 132:37715
TI Spontaneous ignition system for gas generating compositions for inflation of automobile airbags
IN Jordan, Michael P.; Rink, Karl K.; Hatt, Wesley L.; Pripps, Steven R.; Lindsey, David W.; Green, David J.; Jackson, Scott A.; Cunningham, Donald J.
PA Autoliv ASP Inc., USA
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19925954	A1	20000105	DE 1999-19925954	19990608
PRAI US 1998-93888	A	19980609		

AB A process and apparatus for ignition of a gas generating composition, such as those that are used in vehicle airbag restraint systems, uses an ignitable gas to ignite the gas generating composition The combustible gas can either be located in the free interior chamber of the gas generator, or it can be in a separated, sealed container, either separated of together with the gas generator material. The ignitable gas consists of: (1) a one fuel gas selected from H2, hydrocarbons, hydrazines, acetylenes, organic peroxides, and oxygen-substituted hydrocarbons, and (2) an oxidizer selected from N2O and O2. The solid gas generating material is selected from metal azides, tetrazoles, triazoles, metal salts of dicyanamides, amine nitrate salts, salts of dilituric acid, and salts of 5-nitroorotic acid. He ignitable gas has a spontaneous ignition temperature of 300-450°F.
IT **17687-24-0D**, 5-Nitroorotic acid, salts
RL: TEM (Technical or engineered material use); USES (Uses)
(gas generating compns. containing; spontaneous ignition system for gas generating compns. for inflation of automobile airbags)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

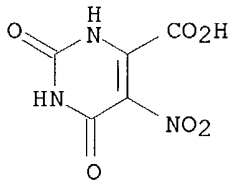


L6 ANSWER 15 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:623692 CAPLUS
DN 132:32548
TI Pyrimidine nucleobase ligands of orotate phosphoribosyltransferase from Toxoplasma gondii
AU Javaid, Z. Z.; el Kouni, M. H.; Iltzsch, M. H.
CS Department of Biological Sciences, University of Cincinnati, Cincinnati, OH, USA
SO Biochemical Pharmacology (1999), 58(9), 1457-1466
CODEN: BCPCA6; ISSN: 0006-2952
PB Elsevier Science Inc.
DT Journal
LA English
AB Sixty-seven pyrimidine nucleobase analogs were evaluated as ligands of Toxoplasma gondii orotate phosphoribosyltransferase (OPRTase, EC 2.4.2.10) by measuring their ability to inhibit this enzyme in vitro. Apparent Ki values were determined for compds. that inhibited T. gondii OPRTase by greater than 20% at a concentration of 400 μM. 1-Deazaorotic acid (0.47 μM) and 5-azaorotic acid (2.1 μM) were found to bind better (8.3- and 1.9-fold, resp.) to T. gondii OPRTase than orotic acid, the natural substrate of the enzyme. Based on these results, a structure-activity relationship of ligand binding to OPRTase was formulated using uracil, barbituric acid, and orotic acid as reference compds. It was concluded that the following structural features of pyrimidine nucleobase analogs were required or strongly preferred for binding: (i) an endocyclic pyridine-type nitrogen or methine at the 1-position; (ii) exocyclic oxo groups at the 2- and 4-positions; (iii) a protonated endocyclic pyridine-type nitrogen at the 3-position; (iv) an endocyclic pyridine-type nitrogen or methine at the 5-position; (v) an exocyclic hydrogen or fluorine at the 5-position; (vi) an endocyclic pyridine-type nitrogen or methine at the 6-position; and (vii) an exocyclic neg. charged or electron-withdrawing group at the 6-position. A comparison of the results from the present study with those from a previous study on mammalian OPRTase [Niedzwicki et al., Biochem Pharmacol 33: 2383-2395, 1984] identified four compds. (6-chlorouracil, 5-azaorotic acid, 1-deazaorotic acid, and 6-iodouracil) that may bind selectively to T. gondii OPRTase.
IT **7164-43-4**, 5-AminoOrotic acid **17687-24-0**, 5-NitroOrotic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(pyrimidine nucleobase ligands of orotate phosphoribosyltransferase from Toxoplasma gondii)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI)

(CA INDEX NAME)



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 16 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:595127 CAPLUS
DN 131:228643
TI Preparation of oxalylaminothiophene derivatives as modulators of protein tyrosine phosphatases (PTPases)
IN Richter, Lutz Stefan; Andersen, Henrik Sune; Vagner, Josef; Jeppesen, Claus Bekker; Moller, Niels Peter Hundahl; Branner, Sven; Jeppesen, Lone; Olsen, Ole Hvilsted; Iversen, Lars Fogh; Holsworth, Daniel Dale; Axe, Frank Urban; Ge, Yu; Jones, Todd Kevin; Ripka, Wiliam Charles; Uyeda, Roy Teruyuki; Su, Jing; Bakir, Farid; Judge, Luke Milburn
PA Novo Nordisk A/S, Den.; Ontogen Corporation; Richter, Birgith
SO PCT Int. Appl., 230 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9946237	A1	19990916	WO 1999-DK126	19990312
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6225329	B1	20010501	US 1999-265069	19990309
	US 2002019412	A1	20020214	US 1999-265316	19990309
	AU 9927139	A1	19990927	AU 1999-27139	19990311
	US 6262044	B1	20010717	US 1999-268490	19990311
	US 2002002199	A1	20020103	US 1999-266395	19990311
	CA 2323472	AA	19990916	CA 1999-2323472	19990312
	ZA 9902029	A	19990927	ZA 1999-2029	19990312
	ZA 9902032	A	19990927	ZA 1999-2032	19990312
	ZA 9902038	A	19990927	ZA 1999-2038	19990312
	ZA 9902036	A	19991001	ZA 1999-2036	19990312
	BR 9908723	A	20001121	BR 1999-8723	19990312
	EP 1080068	A1	20010307	EP 1999-907336	19990312
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, FI, RO				
	JP 2004500308	T2	20040108	JP 2000-535620	19990312
	NO 2000004526	A	20001108	NO 2000-4526	20000911
	US 6410586	B1	20020625	US 2001-810266	20010316
	US 2002165398	A1	20021107	US 2002-127043	20020419
	US 2003069267	A1	20030410	US 2002-158464	20020528
PRAI	DK 1998-350	A	19980312		
	DK 1998-345	A	19980312		
	DK 1998-343	A	19980312		
	DK 1998-342	A	19980312		
	DK 1998-344	A	19980312		
	DK 1998-347	A	19980312		
	DK 1998-346	A	19980312		
	DK 1998-348	A	19980312		
	DK 1998-479	A	19980403		
	DK 1998-472	A	19980403		
	DK 1998-473	A	19980403		

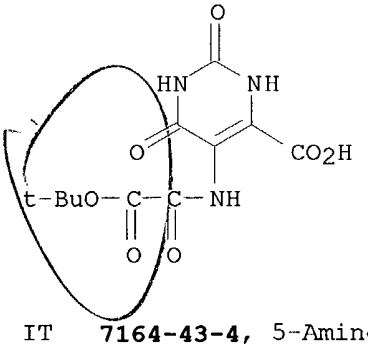
DK 1998-478	A	19980403
DK 1998-475	A	19980403
DK 1998-474	A	19980403
DK 1998-476	A	19980403
DK 1998-480	A	19980403
US 1998-82912P	P	19980424
DK 1998-667	A	19980515
US 1998-88115P	P	19980605
DK 1998-939	A	19980715
DK 1998-940		19980715
DK 1998-938		19980715
DK 1998-1385		19981028
DK 1998-1561		19981126
DK 1998-1612		19981207
US 1998-82365P	P	19980420
US 1998-82368P	P	19980420
US 1998-82371P	P	19980420
US 1998-82373P	P	19980420
US 1998-82913P	P	19980424
US 1998-82914P	P	19980424
US 1998-82915P	P	19980424
US 1998-93525P	P	19980721
US 1998-93620P	P	19980721
US 1998-93638P	P	19980721
US 1998-108747P	P	19981117
US 1999-115528P	P	19990112
US 1999-266395	B1	19990311
US 1999-268490	A3	19990311
WO 1999-DK126	W	19990312
US 2001-810266	A3	20010316

AB Oxalylaminoheterocycles (e.g., oxalylaminothiophene and oxalylaminothienopyran derivs., etc.) were prepared as inhibitors of Protein Tyrosine Phosphatases (PTPases), such as PTP1B, TC-PTP, CD45, SHP-1, SHP-2, PTPα, PTPε, PTPμ, PTPδ, PTPσ, PTPζ, PTPβ, PTPD1, PTPD2, PTPH1, PTP-MEG1, PTP-LAR, and HePTP. These compds. are indicated in the management or treatment of a broad range of diseases such as autoimmune diseases, acute and chronic inflammation, osteoporosis, various forms of cancer and malignant diseases, and type I diabetes and type II diabetes. For instance, 2-amino-5-hydroxymethyl-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid tert-Bu ester (preparation given) was reacted with phthalimide in THF, PPh3, and DIAD to form the 5-phthalimidomethyl derivative (47%). The amine was amidated with imidazol-1-yloxoacetic acid tert-Bu ester in CH2Cl2 and TEA (99%), followed by hydrolysis of the ester function with TFA in CH2Cl2, to give 5-(1,3-dioxo-1,3-dihydroisoindol-2-ylmethyl)-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid (I) in 57% yield. In an in vitro test against PTP1B expressed in E. coli and purified by known methods, Ki values at various inhibitor concns. were determined An anal. of selectivity of two PTPase inhibitors against PTP1B, PTP-LAR, PTPε, CD45, and PTPβ showed that one compound of the invention is a non-selective inhibitor, whereas another behaves like a selective inhibitor.

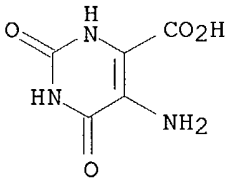
IT **243990-00-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of oxalylaminothiophene derivs. as modulators of protein tyrosine phosphatases (PTPases))

RN 243990-00-3 CAPLUS

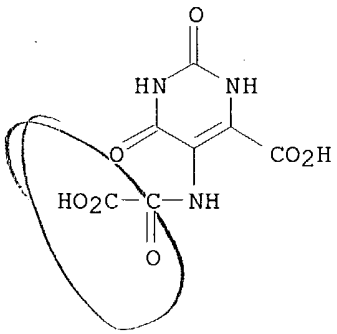
CN 4-Pyrimidinecarboxylic acid, 5-[[(1,1-dimethylethoxy)oxoacetyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of oxalylaminothiophene derivs. as modulators of protein tyrosine phosphatases (PTPases))
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **243989-99-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of oxalylaminothiophene derivs. as modulators of protein tyrosine phosphatases (PTPases))
RN 243989-99-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(carboxycarbonyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 17 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:595124 CAPLUS
DN 131:228549
TI Preparation of (oxalylamino)benzoic acid derivatives and analogs as modulators of protein tyrosine phosphatases (PTPases)
IN Richter, Lutz Stefan; Andersen, Henrik Sune; Vagner, Josef; Jeppesen, Claus Bekker; Moller, Niels Peter Hundahl; Branner, Sven; Su, Jing; Bakir, Farid; Judge, Luke Milburn
PA Novo Nordisk A/S, Den.; Ontogen Corporation
SO PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9946236	A1	19990916	WO 1999-DK122	19990311
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6225329	B1	20010501	US 1999-265069	19990309
	AU 9927136	A1	19990927	AU 1999-27136	19990311
	EP 1062199	A1	20001227	EP 1999-907333	19990311
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2002506055	T2	20020226	JP 2000-535619	19990311
	ZA 9902029	A	19990927	ZA 1999-2029	19990312
PRAI	DK 1998-342	A	19980312		
	DK 1998-345	A	19980312		
	DK 1998-472	A	19980403		
	DK 1998-479	A	19980403		
	DK 1998-940	A	19980715		
	US 1998-82913P	P	19980424		
	US 1998-82914P	P	19980424		
	US 1998-93638P	P	19980721		
	WO 1999-DK122	W	19990311		

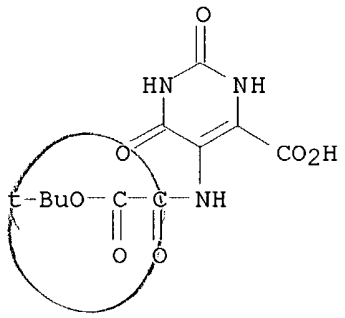
OS MARPAT 131:228549
AB Title compds. I [A = atoms to complete (un)substituted Ph, biphenyl, indenyl, fluorenyl, naphthyl, pyridyl, pyridazinyl, pyrimidinyl, or pyrazinyl nucleus; R1 = H, acyl, CO2H, OH or derivs., CF3, NO2, cyano, SO3H, amino, various 5-membered heterocycles, etc.; R2 = acyl, CO2H, OH or derivs., CF3, NO2, cyano, SO3H, (un)substituted NH2 or PO3H2, various 5-membered heterocycles, etc.; R4 = H, OH, alkyl, (un)substituted aryl or aralkyl, (un)substituted NH2, alkoxy] were prepared as inhibitors of protein tyrosine phosphatases (PTPases), such as PTP1B, CD45, SHP-1, SHP-2, PTPα, LAR, and HePTP. The compds. are useful in the treatment of type I diabetes, type II diabetes, impaired glucose tolerance, insulin resistance, obesity, immune dysfunctions including autoimmunity diseases with dysfunctions of the coagulation system, allergic diseases including asthma, osteoporosis, proliferative disorders including cancer and psoriasis, diseases with decreased or increased synthesis or effects of growth hormone, diseases with decreased or increased synthesis of hormones or cytokines that regulate the release of/or response to growth hormone,

diseases of the brain including Alzheimer's disease and schizophrenia, and infectious diseases. For instance, anthranilic acid was amidated with Et oxalyl chloride in THF (94%), followed by hydrolysis of the ester function with NaOH in aqueous EtOH solution (81%), to give the title compound II. In an in vitro test against PTP1B expressed in E. coli and purified by known methods, II had a Ki of 20 μM, and the similarly prepared 2,3-substituted naphthalene analog III had a Ki of 9.9 μM.

IT **243990-00-3P**, 5-[(tert-Butoxyoxalyl)amino]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (oxalylamino)benzoic acid derivs. and analogs as modulators of protein tyrosine phosphatases (PTPases))

RN 243990-00-3 CAPLUS

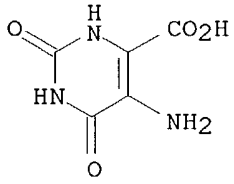
CN 4-Pyrimidinecarboxylic acid, 5-[[(1,1-dimethylethoxy)oxoacetyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of (oxalylamino)benzoic acid derivs. and analogs as modulators of protein tyrosine phosphatases (PTPases))

RN 7164-43-4 CAPLUS

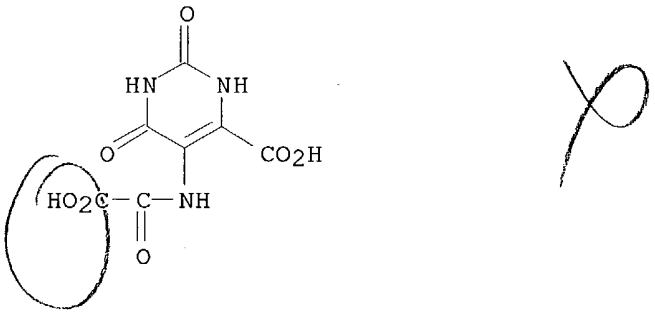
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **243989-99-3P**, 5-(Oxalylamino)-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of (oxalylamino)benzoic acid derivs. and analogs as modulators of protein tyrosine phosphatases (PTPases))

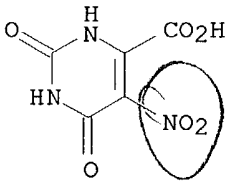
RN 243989-99-3 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-[(carboxycarbonyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



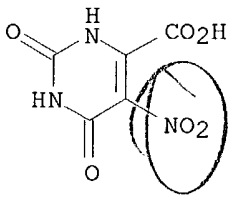
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:376615 CAPLUS
DN 131:214115
TI C=O stretching frequencies in some nucleic acid base derivatives: part I
AU Mital, H. P.; Bhardwaj, S.; Singhal, S. K.; Sharma, R. K.
CS Department of Physics, Meerut College, Meerut, India
SO Asian Chemistry Letters (1997), 1(2-4), 77-80
CODEN: ACLEFK
PB Anita Publications
DT Journal
LA English
AB The carbonyl stretching region is some some what peculiar and v (C=O) modes are the most important modes of nucleic acid base derivs., because they take part in hydrogen bonding. The present study reports a comparison of C=O stretching frequencies in different nucleic acid base derivs.
IT **17687-24-0,** 5-Nitroorotic acid
RL: PRP (Properties)
(C=O stretching frequencies in some nucleic acid base derivs.)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



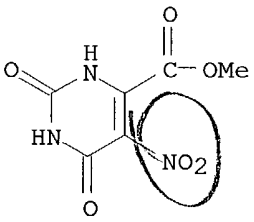
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 19 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:304467 CAPLUS
DN 131:18989
TI Effect of A-ring modifications on the DNA-binding behavior and cytotoxicity of pyrrolo[2,1-c][1,4]benzodiazepines
AU Thurston, David E.; Bose, D. Subhas; Howard, Philip W.; Jenkins, Terence C.; Leoni, Alberto; Baraldi, Pier G.; Guiotto, Andrea; Cacciari, Barbara; Kelland, Lloyd R.; Foloppe, Marie-Paule; Rault, Sylvain
CS CRC Gene Targeted Drug Design Research Group School of Pharmacy and Biomedical Sciences, University of Portsmouth, Portsmouth Hants, P01 2DT, UK
SO Journal of Medicinal Chemistry (1999), 42(11), 1951-1964
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Several A-ring-modified analogs of the DNA-binding antitumor agent DC-81 I (R = H, R1 = Me) have been synthesized in order to study structure-reactivity/cytotoxicity relationships. For two mols., the modifications required the addition of a fourth ring to give the novel dioxolo[4,5-h]- and dioxano[5,6-h]pyrrolo[2,1-c][1,4]benzodiazepin-11-one (PBD) ring systems, resp. Another three analogs have the native benzenoid A-ring replaced with pyridine, diazine, or pyrimidine rings to give the novel pyrrolo[2,1-c][1,4]pyridodiazepine, pyrrolo[2,1-c][1,4]diazinodiazepine, and pyrrolo[2,1-c][1,4]pyrimidinodiazepine systems, resp. The other new analogs have extended chains at the C8-position of the DC-81 structure. During the synthesis of these compds., a novel tin-mediated regiospecific cleavage reaction of the dioxole intermediate II was discovered, leading to the previously unknown iso-DC-81 I (R = Me, R1 = H). In addition, an unusual simultaneous nitration-oxidation reaction of 4-(3-hydroxypropoxy)-3-methoxybenzoic acid was found to produce 3-(4-carboxy-2-methoxy-5-nitrophenoxy)propanoic acid, a key intermediate, in high yield. In general, the results of cytotoxicity and DNA-binding studies indicated that none of the changes made to the A-ring of the PBD system significantly improved either binding affinity or cytotoxicity in comparison to DC-81. This result suggests that the superior potency of natural products such as anthramycin, tomaymycin, and sibiromycin is due entirely to differences in C-ring structure, and in particular exo or endo unsatn. at the C2-position and C2-substituents containing unsatn. This study also provided information regarding the influence of A-ring substitution pattern on the relative stability of the interconvertible N10-C11 carbinolamine, carbinolamine Me ether, and imine forms of PBDs.
IT **65717-13-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, cytotoxicity, and DNA-binding behavior of pyrrolobenzodiazepines)
RN 65717-13-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, monopotassium salt (9CI) (CA INDEX NAME)



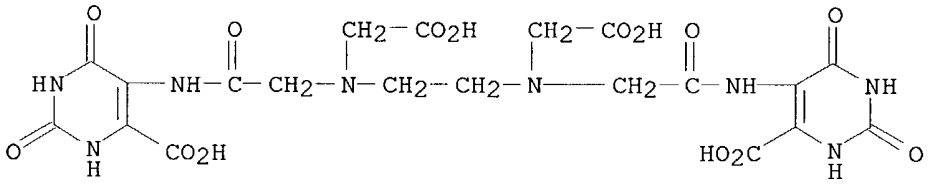
● K

IT **6311-73-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, cytotoxicity, and DNA-binding behavior of pyrrolobenzodiazepines)
RN 6311-73-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 20 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:302297 CAPLUS
DN 129:61955
TI Synthesis and characterization of chelating polycarboxylate ligands capable of forming intermolecular, complementary triple hydrogen bonds
AU Ulvenlund, Stefan; Georgopoulou, Alexandra S.; Mingos, D. Michael P.; Baxter, Ian; Lawrence, Simon E.; White, Andrew J. P.; Williams, David J.
CS Department of Chemistry, Imperial College of Science, Technology and Medicine, London, SW7 2AY, UK
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (11), 1869-1878
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB The reaction between the dianhydride of ethylenedinitrilotetraacetic acid (EDTA) (1) and aminouracil derivs. was utilized to synthesize bifunctional, chelating ligands capable of coordinating to a metal center via the EDTA backbone, while simultaneously being able to form complementary intermol. H bonds via the uracil moieties. 5-Aminouracil (2), 5-aminoorotic acid (3), 5,6-diaminouracil (4) and 5,6-diamino-2-thiouracil (5) were treated with 1 in dry DMF or DMSO to give functionalized dicarboxamide derivs. H2L1-H2L4 in 15-90% yield. 4 And 5 reacted with the dianhydride exclusively via the 5-amino position. The reaction of H2L1 and H2L3 with basic metal salts KVO3 and Zn(O2CMe)2 in aqueous solns. gave metal complexes of the anionic ligands L1-L4: K[VO2L1]·5H2O, [Zn(OH2)L1]·4H2O and [Zn(OH2)L3]·5H2O which were characterized by single-crystal x-ray crystallog. The solid state structures of these complexes show that the uracil moieties are situated on pendant side-arms. The high degree of rotational freedom of these H-bonding groups makes this class of metal complex promising in terms of specific binding to water-soluble biomols. having complementary H-bonding sites. [Zn(OH2)L1] and [NiL1]·3H2O were also synthesized.
IT **208533-61-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 208533-61-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5,5'-[1,2-ethanediylbis[[(carboxymethyl)imino](1-oxo-2,1-ethanediyl)imino]]bis[1,2,3,6-tetrahydro-2,6-dioxo-, tetrahydrate (9CI) (CA INDEX NAME)



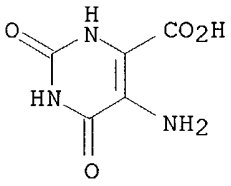
● 4 H_2O

IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with ethylenedinitrilotetraacetic acid dianhydride)

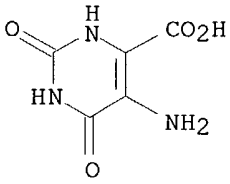
RN 7164-43-4 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 21 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:203872 CAPLUS
DN 128:330266
TI New metal-binding modes for 5-aminoorotic acid: preparation, characterization and crystal structures of zinc(II) complexes
AU Lalioti, Nikolia; Raptopoulou, Catherine P.; Terzis, Aris; Panagiotopoulos, Athanassios; Perlepes, Spyros P.; Manessi-Zoupa, Evy
CS Department of Chemistry, University of Patras, Patras, 265 00, Greece
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (8), 1327-1334
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB Treatment of ZnCl2 with 2 equiv of 5-aminoorotic acid (5-amino-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid, H4L) and 2 equiv of NaOH in water-MeOH yielded a mixture of crystals and powder of {Zn(H2L)(H2O)2}n (1) and [Zn(H3L)2(H2O)4] (2), resp. A good yield (.apprx.70%) of pure 2 can be obtained by the reaction of Zn(O2CMe)2·2H2O and 2 equiv of H4L in refluxing H2O. The crystal structure of 1 consists of neutral octahedral [Zn(H2L)(H2O)2] units which form polymer chains along the b axis; H2L2- behaves as a bis(bidentate) bridging ligand coordinating to two Zn atoms via the amino N, the O of the neutral carboxamide group, the deprotonated carboxamide N and one of the carboxylate oxygens and forming two five-membered chelate rings. The 1H NMR spectra of 1 in (CD3)2SO at 290 and 310 K suggest that its solid-state structure is not retained in solution Slow crystallization of 1 or 2 from DMSO solns. yielded crystals of the monomeric octahedral complex [Zn(H3L)2(DMSO)2(H2O)2] (3) the structure of which was solved by single-crystal x-ray crystallog. The monoanion H3L- uses only one carboxylate O for metal binding in the centrosym. complex 3. The difference in anionic charge and coordination mode between H2L2- and H3L- leads to different H-bonded supramol. structures for 1 and 3. The IR and 1H NMR spectra of the prepared complexes are discussed.
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with zinc)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



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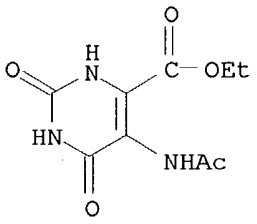
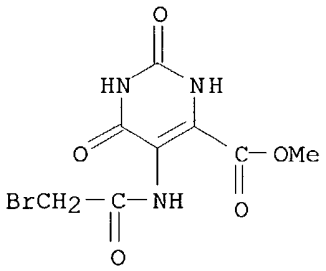
RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

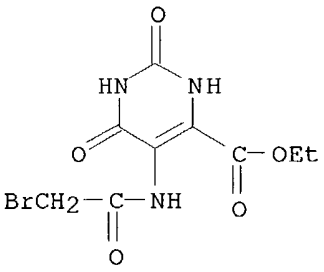
L6 ANSWER 22 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:191978 CAPLUS
DN 128:319227
TI Antibacterial activity of 5-aminoorotic acid derivatives
AU El Kolli, M.; Coulibaly, A.; Chevalier, J.; Barbe, J.; Cremieux, A.
CS GERCTOP-ESA CNRS 6009, Faculte de Pharmacie, Marseille, 13385, Fr.
SO Current Microbiology (1998), 36(4), 245-247
CODEN: CUMIDD; ISSN: 0343-8651
PB Springer-Verlag New York Inc.
DT Journal
LA English
AB The antibacterial activity of several new 5-aminoorotic acid derivs. considered as possible competitors of orotate towards dihydroorotase has been investigated. Products with a bromacetamido substitution demonstrated antibacterial properties. However, the paradoxical behavior of some compds. in synthetic media, opposed to the expected results obtained with an E. coli strain lacking dehydroorotic dehydrogenase, did not allow us to draw conclusions on their mechanism of action.
IT **40598-10-5 187232-28-6 187232-29-7 187232-30-0 187232-31-1 187232-32-2 187232-33-3 187232-34-4 187232-35-5 187232-36-6 187232-38-8 187232-39-9 187232-40-2 187232-41-3 207237-31-8 207237-32-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antibacterial activity of 5-aminoorotic acid derivs.)
RN 40598-10-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



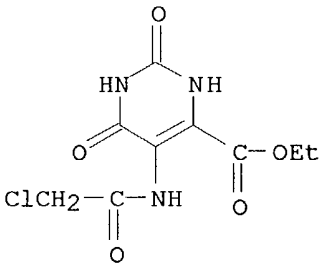
RN 187232-28-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



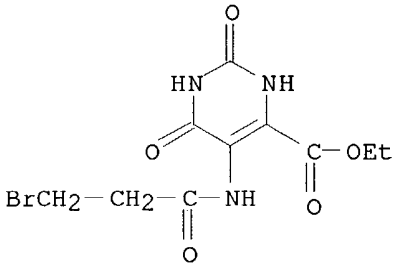
RN 187232-29-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



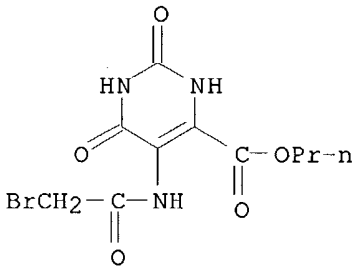
RN 187232-30-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



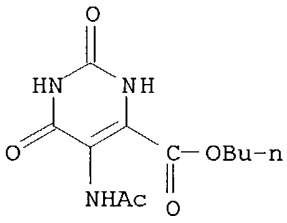
RN 187232-31-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



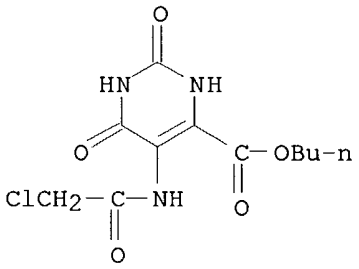
RN 187232-32-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, propyl ester (9CI) (CA INDEX NAME)



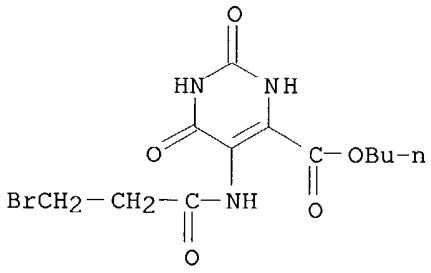
RN 187232-33-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



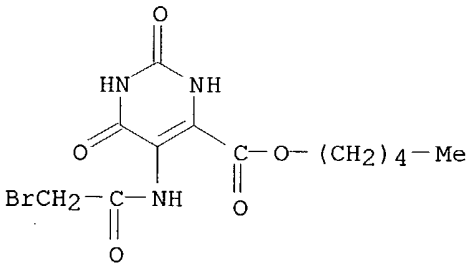
RN 187232-34-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



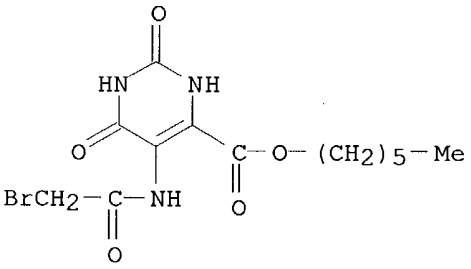
RN 187232-35-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



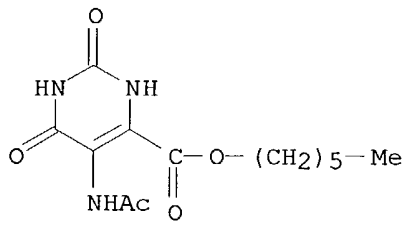
RN 187232-36-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, pentyl ester (9CI) (CA INDEX NAME)



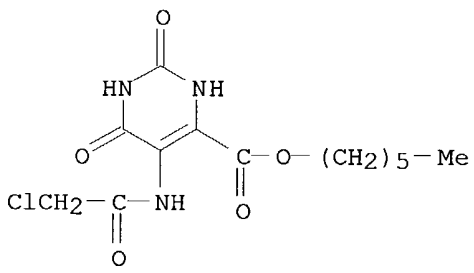
RN 187232-38-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



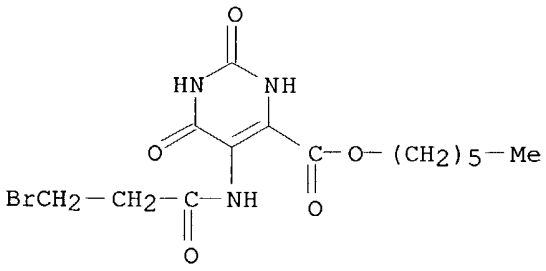
RN 187232-39-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



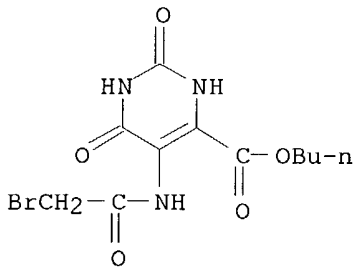
RN 187232-40-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



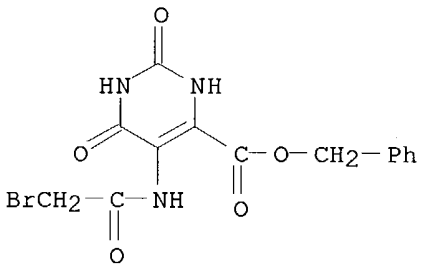
RN 187232-41-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



RN 207237-31-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



RN 207237-32-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

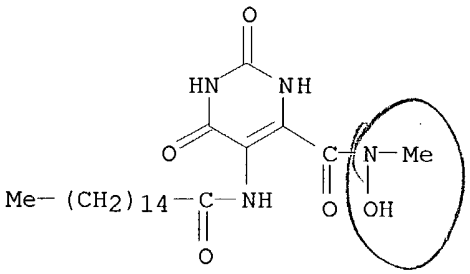
L6 ANSWER 23 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:210662 CAPLUS
DN 126:205416
TI Silver halide photographic material with improved shelf life and latent image stability and a hydroxamic acid to be used for the material
IN Mikoshiba, Takashi; Takizawa, Hiroo; Hosokawa, Junichiro; Ishii, Yoshio; Obayashi, Keiji; Morigaki, Masakazu
PA Fuji Photo Film Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 76 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 09005920	A2	19970110	JP 1995-172969	19950616
PRAI JP 1995-172969		19950616		

AB Claimed photog. material contains a hydroxamic acid R2C(:O)NR1OH (I; R1 = H, C1-30 alkyl; R2 = heterocyclic group having C≥7 atoms). Preferable R2 is pyridyl and 4-piperidinyl, and the compds. I itself is claimed, too. The hydroxamic acid improves the storage stability and latent image stability of the photog. material, particularly of multilayer high speed camera films. Suitable compds. to be added to the emulsion layer are compound I with (R1 = Me; R2 = 3-(2-octyl-2-decyl-ethoxycarbonyl)pyridine-2-1), (R1 = Me; R2 = 3-(hexadecyloxycarbonyl)pyridine-2-yl), (R1 = Me; R2 = N-(heptadecyleneicosylaceto)piperidin-4-yl), etc.

IT **187840-29-5**
RL: DEV (Device component use); USES (Uses)
(photog. materials containing hydroxamic acids for improved shelf life and latent image stability for high-speed camera films)

RN 187840-29-5 CAPLUS
CN 4-Pyrimidinecarboxamide, 1,2,3,6-tetrahydro-N-hydroxy-N-methyl-2,6-dioxo-5-[(1-oxohexadecyl)amino]- (9CI) (CA INDEX NAME)

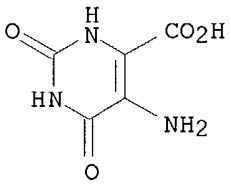


L6 ANSWER 24 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:207630 CAPLUS
DN 126:199931
TI Olefin (co)polymerization process, catalysts therefor and their preparation
IN Johnson, Lynda Kaye; Feldman, Jerald; Kreutzer, Kristina Ann; McLain, Stephan James; Bennett, Alison Margaret Anne; Coughlin, Edward Bryan; Donald, Dennis Scott; Nelson, Lissa Taka Jennings; Parthasarathy, Anju; Shen, Xing; Tam, Wilson; Wang, Yueli; et al.
PA E. I. Du Pont de Nemours & Co., USA
SO PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9702298	A1	19970123	WO 1996-US11131	19960628
	W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, US, UZ, VN, AM, AZ, BY				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5714556	A	19980203	US 1996-671392	19960627
	CA 2225246	AA	19970123	CA 1996-2225246	19960628
	AU 9664040	A1	19970205	AU 1996-64040	19960628
	AU 703202	B2	19990318		
	EP 835269	A1	19980415	EP 1996-923561	19960628
	R: AT, BE, DE, DK, ES, FR, GB, LU, NL, SE, PT, IE, FI				
	CN 1194653	A	19980930	CN 1996-196662	19960628
	CN 1133659	B	20040107		
	BR 9609635	A	19990518	BR 1996-9635	19960628
	JP 11508635	T2	19990727	JP 1996-505255	19960628
	US 6103920	A	20000815	US 1997-899032	19970723
	NO 9706120	A	19980302	NO 1997-6120	19971229
PRAI	US 1995-747P	P	19950630		
	US 1996-671392	A1	19960627		
	WO 1996-US11131	W	19960628		

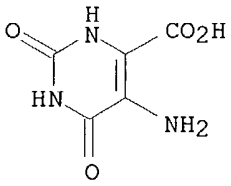
OS MARPAT 126:199931
AB Ethylene, norbornenes and/or styrenes are polymerized under various conditions by contacting in a solution of a zero valent tricoordinate or tetracoordinate nickel compound which has ≥1 labile ligand (all ligands are neutral), an HX acid (X = BF4-, PF6-, etc.), and a compound which is or can be coordinated to the nickel. The polymers produced are useful for films, molding resins, and elastomers. Thus, 0.060 g tetrakis[3,5-bis(trifluoromethyl)phenyl]borate bis(diethyletherate) was added to a mixture of 0.017 g bis(η4-1,5-cyclooctadienyl)nickel and 0.023 g compound I 0.023 in 5.0 mL benzene, the solution frozen, thawed under ethylene atmospheric, and agitated under 6.9 MPa C2H4 for 18 h at 25° to give 9.1 g polyethylene having a very broad m.p. at .apprx.0° and a sharp m.p. at 115°.
IT **7164-43-4**
RL: CAT (Catalyst use); USES (Uses)
(catalyst component; olefin (co)polymerization process and catalysts therefor)

RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as # 21

L6 ANSWER 26 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:634355 CAPLUS
DN 125:315232
TI 5-Aminoorotic acid, a versatile ligand with the ability to exhibit differing coordination and hydrogen-bonding modes: synthesis and crystal structures of platinum(II) complexes
AU Burrows, Andrew D.; Mingos, D. Michael P.; White, Andrew J. P.; Williams, David J.
CS Dep. Chem., Imperial Coll. Sci., Tech. and Med., South Kensington, SW7 2AY, UK
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (19), 3805-3812
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB [Pt(cod)Cl2] (cod = cycloocta-1,5-diene, C8H12) reacted with 2 equiv of PPh3 and an excess of 5-aminoorotic acid (5-amino-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid, H4L) in the presence of silver(I) oxide to give two isomers of [Pt(PPh3)3(H2L)] (1 and 2). 1 And 2 can be separated by fractional crystallization but, in CDCl3 solution, each slowly converts into an equilibrium mixture of the two. Crystal structure detns. showed that in both 1 and 2 the 5-aminoorotate ligand coordinates to the platinum atom as a dianion. In 1 this is achieved via deprotonation of the carboxylic acid and the loss of an amino NH2 proton, leading to a six-membered chelate ring, whereas in 2 it is by deprotonation of the carboxylic acid and loss of the amido proton, leading to a five-membered chelate ring. This difference in coordination mode leads to a difference in the orientation of the hydrogen-bond donors and acceptors remaining on the ligand which, in turn, leads to different supramol. structures, dimers for 1 and tetramers for 2, with the latter structurally similar to guanine tetrads. These naturally occurring units are stabilized by alkali-metal ions, but reaction of 2 with a compound such as NaBF4 in a two-phase dichloromethane-water system led to [Pt2(PPh3)4(HL)][BF4] as the only platinum-containing product. A crystal structure determination showed that in this complex the ligand is trianionic, deprotonated at the carboxylic acid and both the amido and amino nitrogen atoms, coordinating to two platinum atoms via five- and six-membered chelate rings. When dppe [1,2-bis(diphenylphosphino)ethane] was used instead of PPh3 only one isomer of [M(dppe)(H2L)] (M = Pt 3 or Pd 4) was observed for both platinum and palladium, containing the five-membered chelate ring.
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of platinum or palladium aminoorotate phosphine complexes)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

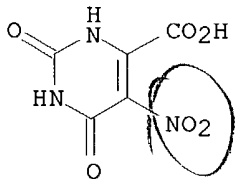
L6 ANSWER 27 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:524278 CAPLUS
DN 125:172649
TI Gas-generating compositions using dicyanamide salts as fuel
IN Barnes, Michael W.; Deppert, Thomas M.; Taylor, Robert D.
PA Morton International, Inc., USA
SO U.S., 4 pp., Cont.-in-part of U.S. Ser. No. 165,771.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5544687	A	19960813	US 1994-182478	19940114
	AU 9475957	A1	19950803	AU 1994-75957	19941020
	AU 668660	B2	19960509		
	CA 2134187	AA	19950611	CA 1994-2134187	19941024
	EP 661253	A2	19950705	EP 1994-308331	19941111
	EP 661253	A3	19950913		
	R: BE, DE, ES, FR, GB, IT, NL, SE				
	JP 07206570	A2	19950808	JP 1994-307341	19941212
	JP 2698553	B2	19980119		
PRAI	US 1993-165771		19931210		
	US 1994-182478		19940114		

AB The compns. comprise approx. 10-60 weight% fuel, .gtorsim.25-100 weight% of which consist of ≥1 transition metal salts of dicyanamide and balance other fuel, and balance ≥1 oxidizers selected from NH4, alkali metal, and alkaline earth chlorates, perchlorates, and nitrates. The preferred transition metal salts of dicyanamide are Zn dicyanamide and Cu dicyanamide. These non-azide propellants are especially suitable for use in automotive air bag restraint systems. A composition containing Cu dicyanamide 26.77, guanidine nitrate 10, Li2CO3 10, and Sr(NO3)2 53.23 weight% had burn rate @ 1000 psi 0.75 in./s and gave 1.70 mol/100 g.

IT **17687-24-0D**, salts
RL: TEM (Technical or engineered material use); USES (Uses)
(fuel; dicyanamide salts as fuel in propellant compns. for airbags)

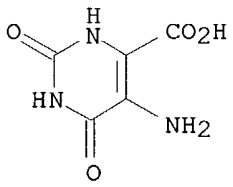
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 28 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:333008 CAPLUS
DN 125:127644
TI Method for obtaining improved image contrast in migration imaging members
IN Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths, Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron, Marie-Eve
PA Xerox Corp., USA
SO U.S., 147 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5514505	A	19960507	US 1995-441360	19950515
	CA 2169980	AA	19961116	CA 1996-2169980	19960221
	CA 2169980	C	20010424		
	JP 08314240	A2	19961129	JP 1996-113456	19960508
	EP 743573	A2	19961120	EP 1996-303359	19960514
	EP 743573	A3	19970305		
	EP 743573	B1	20000906		
	R: DE, FR, GB				
PRAI	US 1995-441360	A	19950515		

OS MARPAT 125:127644
AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.
IT **7164-43-4**, 5-Aminoorotic acid
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(transparentizing agent for electrophotog. migration imaging members)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

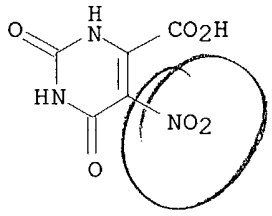
L6 ANSWER 29 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:228497 CAPLUS
DN 124:260710
TI Production of 5-nitroorotic acid
IN Aldea, Vasilichia; Lefter, Emilia; Ardeleanu, Aurelia; Jegu, Constanta; Rosu, Nuta
PA Intreprinderea de Medicamente, Bucuresti, Rom.
SO Rom., 3 pp.
CODEN: RUXXA3
DT Patent
LA Romanian
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI RO 104719	B1	19940930	RO 1989-141202	19890809
PRAI RO 1989-141202		19890809		

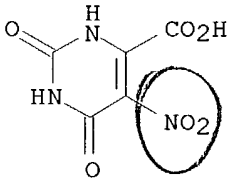
AB 5-Nitroorotic acid for use in the preparation of dipiridamol is manufactured by oxidative nitration of 4-methyluracil with a mixture of 55-60% HNO3-concentrated H2SO4 in a ratio of 1:3.5:3 at 73-76 °. The yield is 70-73%.

IT **17687-24-0P**, 5-Nitroorotic acid
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of nitroorotic acid)

RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 30 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:10546 CAPLUS
DN 124:133867
TI New polynuclear manganese(II) complexes with orotic acid and some of its derivatives: crystal structures, spectroscopic and magnetic studies
AU Nepveu, Francoise; Gaultier, Nicolas; Korber, Kikolaus; Jaud, Joel; Castan, Paule
CS Universite Paul Sabatier, Toulouse, 31062, Fr.
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (24), 4005-13
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB Three polynuclear Mn(II) complexes containing orotic acid (2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid, H3L1) or one of its substituted derivs. [1-methyl- (H2L2) or 5-nitro-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (H3L3)] were synthesized and characterized by x-ray crystallog., UV/visible and magnetic susceptibility measurements. Complex 1 consists of neutral [Mn2(HL1)2(H2O)6] units, which form polymer chains along the z axis with a Mn(1)...Mn(2) distance in the unit cell of 5.628(1) Å while the Mn(2)...Mn(2) distance in the chain is 4.715(1) Å. Each unit cell of complex 2 contains one neutral centrosym. dimer [Mn2(L2)2(H2O)6] containing a short Mn...Mn distance [3.472(2) Å] and an antiferromagnetic exchange interaction is present. The exptl. data were fitted to the susceptibility equations resulting from the Hamiltonian H = -2JS1S2 to give exchange parameter J = -1.3 cm-1 and g = 1.95. From EPR spectra of 2, the hyperfine interaction parameter A = -0.27 GHz and the zero-field splitting parameter D = ±2.93 GHz were calculated Each unit cell of 3 consists of one dinuclear anion [Mn2(HL3)2(H2O)4Cl2]2- and of one cation [K2(H2O)]2+. The Mn(1) and Mn(2) atoms and the H2O mol. of [K2(H2O)]2+ are situated at inversion sites. The dinuclear anions are associated to form chains but the shortest Mn...Mn distance of 5.642(3) Å is observed within the [Mn2(HL3)2(H2O)4Cl2]2- unit between Mn(1) and Mn(2).
IT **65717-13-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with manganese chloride)
RN 65717-13-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, monopotassium salt (9CI) (CA INDEX NAME)



● K

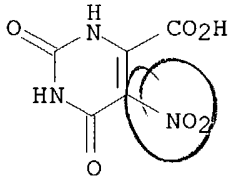
L6 ANSWER 31 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:938295 CAPLUS
DN 123:318130
TI Gas generating compositions with alkali oxide scavengers
IN Taylor, Robert D.; Deppert, Thomas M.
PA Morton International, Inc., USA
SO Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 678492	A1	19951025	EP 1995-301693	19950314
	R: BE, DE, ES, FR, GB, IT, NL, SE				
	AU 9513426	A1	19951116	AU 1995-13426	19950223
	CA 2143360	AA	19951019	CA 1995-2143360	19950224
	JP 08034693	A2	19960206	JP 1995-55878	19950315
PRAI	US 1994-228983		19940418		

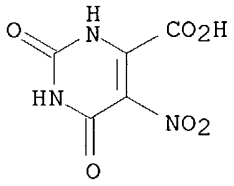
AB A gas generating composition used for airbag restraint systems encased in an aluminum housing comprises a fuel selected from 5-nitrobarbituric acid (or its salts), 5-nitroorotic acid (or its salt); an oxidizer selected from chlorate, perchlorate, or nitrate of ammonium, alkali metal, and/or alkaline earth metal and/or a transition metal oxide such as cupric oxide, alumina, and/or silica; and a binder.

IT **17687-24-0**, 5-Nitroorotic acid **65717-13-7**
RL: NUU (Other use, unclassified); TEM (Technical or engineered material use); USES (Uses)
(gas generating compns. with alkali oxide scavengers)

RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 65717-13-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, monopotassium salt (9CI) (CA INDEX NAME)

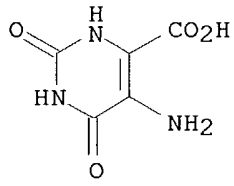


● K

L6 ANSWER 32 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:858608 CAPLUS
DN 123:256757
TI Preparation of indolo[2,1-b]quinazoline-6,12-dione tuberculostatics
IN Baker, William R.; Mitscher, Lester A.
PA Pathogenesis Corp., USA
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

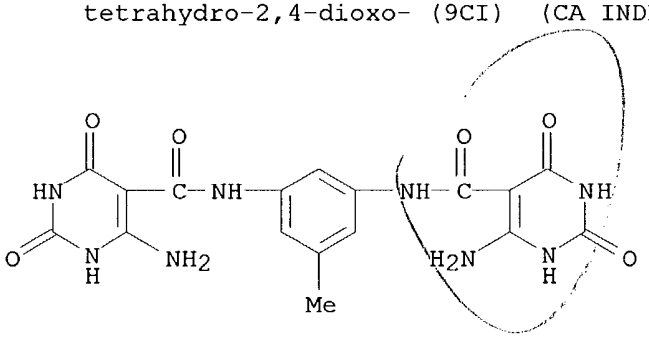
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9513807	A1	19950526	WO 1994-US13259	19941117
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ				
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5441955	A	19950815	US 1993-154784	19931119
	AU 9512100	A1	19950606	AU 1995-12100	19941117
PRAI	US 1993-154784		19931119		
	WO 1994-US13259		19941117		

OS MARPAT 123:256757
AB The title compds. [I; A-H = C, N; or A and B or C and D can be taken together to be N or S; R1-R4, R8, R10 = H, halogen, alkyl, cycloalkyl, (un)substituted heterocyclyl, (un)substituted amino, NO2, CN, CHO, etc.; R7, R9 = H, halogen, (un)substituted alkyl, cycloalkyl, (un)substituted heterocyclyl] useful for the treatment of multidrug-resistant Mycobacterium tuberculosis and M. leprae, are prepared Thus, 5-fluoroisatin was added to a solution of Me3COK and N-methylpyrrolidone, producing 8-fluoroindolo[2,1-b]quinazoline-6,12-dione, II, m.p. 273-276°, which demonstrated a MIC against multiple drug-resistant M. tuberculosis (10038) of <1 μg/mL, vs. 10 μg/mL for tryptanthrin.
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indolo[2,1-b]quinazoline-6,12-dione tuberculostatics from)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

L6 ANSWER 33 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:830218 CAPLUS
DN 124:86949
TI Behavior of toluene diisocyanate towards nucleophiles: Synthesis of some new azoles and azines
AU Moustafa, Hamed Y.
CS Faculty Science, Zagazig University, Egypt
SO Zagazig Journal of Pharmaceutical Sciences (1994), 3(3A), 142-6
CODEN: ZJPSEV; ISSN: 1110-5089
PB University of Zagazig, Faculty of Pharmacy
DT Journal
LA English
AB Toluene diisocyanate was treated with active methylenes to give anilides. The reaction of these anilides with hydrazine gave pyrazoles.
IT **172361-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 172361-89-6 CAPLUS
CN 5-Pyrimidinecarboxamide, N,N'-(5-methyl-1,3-phenylene)bis[6-amino-1,2,3,4-tetrahydro-2,4-dioxo- (9CI) (CA INDEX NAME)

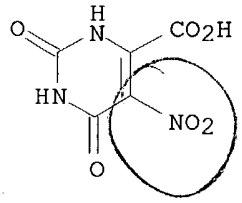


L6 ANSWER 34 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:714018 CAPLUS
DN 123:87614
TI Gas generating composition containing mixed fuels
IN Taylor, Robert D.; Deppert, Thomas M.
PA Morton International, Inc., USA
SO Eur. Pat. Appl., 4 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 661252	A2	19950705	EP 1994-308329	19941111
	R: BE, DE, ES, FR, GB, IT, NL, SE				
	AU 9475956	A1	19950727	AU 1994-75956	19941020
	AU 663659	B2	19951012		
	CA 2134188	AA	19950611	CA 1994-2134188	19941024
	JP 07206569	A2	19950808	JP 1994-306305	19941209
PRAI	US 1993-165273		19931210		

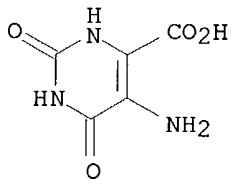
AB A gas generating composition comprises 30-65 weight% fuel and 35-65 weight% oxidizer, and 5-75 weight% of the fuel is selected from aminotetrazole, tetrazole, bitetrazole, and triazole and 25-95 weight% of the fuel is selected from alkali metal and/or alkaline earth metal salts of 5-nitrobarbituric acid and/or 5-nitroorotic acid. The composition is suitable for the inflation of airbags.

IT **60779-49-9**
RL: NUU (Other use, unclassified); USES (Uses)
(gas generating composition containing mixed fuels)
RN 60779-49-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, potassium salt (9CI) (CA INDEX NAME)



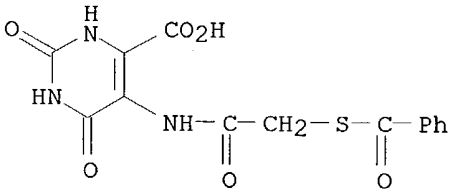
●x K

L6 ANSWER 35 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:524213 CAPLUS
DN 123:46632
TI Technetium and rhenium complexes of derivatized nucleic acid components. 2. Technetium complexes of 5-mercaptoacetylamino orotic acid (MAOA)
AU Noll, St.; Noll, B.; Spies, H.; Dinkelborg, L.; Semmler, W.
CS Inst. Diagnostikforschung, Berlin, Germany
SO Forschungszent. Rossendorf, [Ber.] FZR (1995), FZR-73, Institute of Bioinorganic and Radiopharmaceutical Chemistry, Annual Report, 1994, 67-70
CODEN: FRBFEU
DT Report
LA English
AB 5-(Mercaptoacetylamino)orotic acid was prepared and reacted with technetium gluconate to form a mixture of possibly isomeric products. The reaction does not go to completion, thus the Tc:ligand ratio could not be determined
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of (mercaptoacetylamino)orotic acid and its technetium complex)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

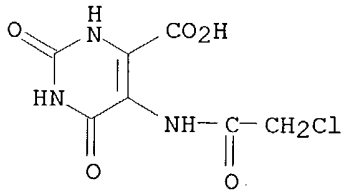


Same as #25

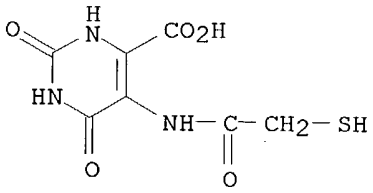
IT **164293-77-0P 164293-78-1P**, 5-(Chloroacetylamino)orotic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of (mercaptoacetylamino)orotic acid and its technetium complex)
RN 164293-77-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[[(benzoylthio)acetyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



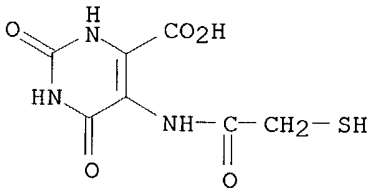
RN 164293-78-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



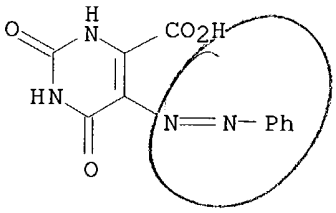
IT **164293-79-2P**, 5-(Mercaptoacetylamino)orotic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with technetium)
RN 164293-79-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(mercaptoacetyl)amino]-2,6-dioxo- (9CI) (CA INDEX NAME)



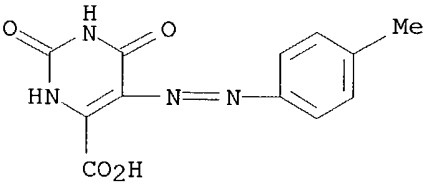
IT **164293-79-2DP**, technetium complex
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 164293-79-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(mercaptoacetyl)amino]-2,6-dioxo- (9CI) (CA INDEX NAME)



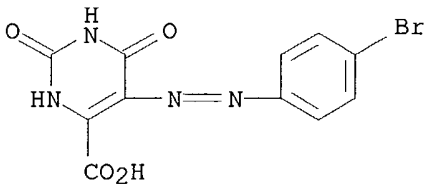
L6 ANSWER 36 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:680180 CAPLUS
DN 121:280180
TI Dissociation constants of arylazo orotic acid compounds and stability constants of their complexes
AU Khalil, Ekram A.; Masoud, Mamdouh S.; El-Merghany, Adel M.
CS Fac. Sci., Alexandria Univ., Alexandria, Egypt
SO Pakistan Journal of Scientific and Industrial Research (1993), 36(2-3), 68-73
CODEN: PSIRAA; ISSN: 0030-9885
DT Journal
LA English
AB Synthesis of new arylazo orotic acids I (R = H, 4-Me, 2-OH, etc.) has been carried out. Values of pKL and log Kc were evaluated. Solvent effects on the thermodn. parameters of dissociation were discussed. The data were explained from the electronic character of the substituents.
IT **155984-14-8DP**, cobalt,copper and nickel complexes
155984-15-9DP, cobalt,copper and nickel complexes
155984-16-0DP, cobalt,copper and nickel complexes
155984-17-1DP, cobalt,copper and nickel complexes
155984-18-2DP, cobalt,copper and nickel complexes
155984-19-3DP, cobalt,copper and nickel complexes
155984-20-6DP, cobalt,copper and nickel complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation constant of)
RN 155984-14-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-(phenylazo)- (9CI) (CA INDEX NAME)



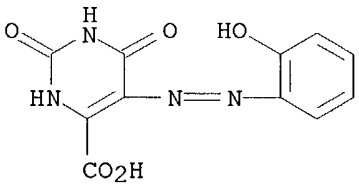
RN 155984-15-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(4-methylphenyl)azo]-2,6-dioxo- (9CI) (CA INDEX NAME)



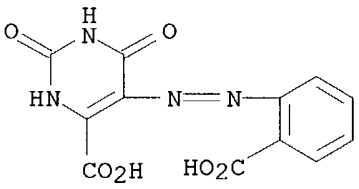
RN 155984-16-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-bromophenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



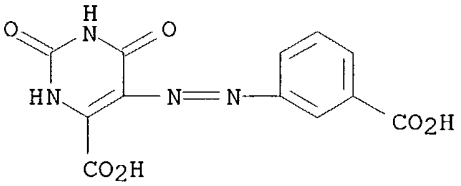
RN 155984-17-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(2-hydroxyphenyl)azo]-2,6-dioxo- (9CI) (CA INDEX NAME)



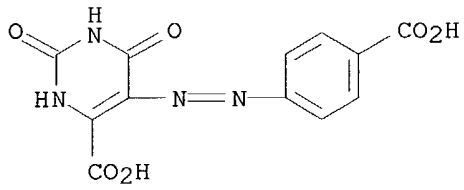
RN 155984-18-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(2-carboxyphenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



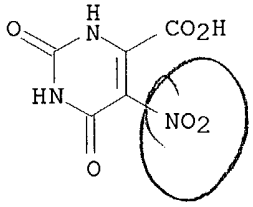
RN 155984-19-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-carboxyphenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



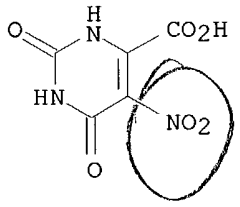
RN 155984-20-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-carboxyphenyl)azo]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 38 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:594977 CAPLUS
DN 121:194977
TI Structure-activity relationship of ligands of uracil phosphoribosyltransferase from Toxoplasma gondii
AU Iltzsch, Max H.; Tankersley, Kevin O.
CS Dep. Biol. Sci., Univ. Cincinnati, Cincinnati, OH, 45221-0006, USA
SO Biochemical Pharmacology (1994), 48(4), 781-91
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB One hundred compds. were evaluated as ligands of Toxoplasma gondii, uracil phosphoribosyltransferase (UPRTase, EC 2.4.2.9) by examining their ability to inhibit this enzyme in vitro. Inhibition was quantified by determining apparent
Ki values fo those compds. that inhibited T. gondii UPRTase by greater than 10% at a concentration of 2 mM. Five compds. (4-thiopyridine, 2-thiopyrimidine, trihiocyanuric acid, 1-deazauracil and 2,4-dithiouracil) bound to the enzyme better than two known substrates for T. gondii UPRTase, 5-fluorouracil and emimycin, which have antitoxoplasmal activity (Pfefferkorn ER, Exp Parasitol 44: 26-35, 1978; Pfefferkorn et al., Exp Parasitol 69: 129-139, 1989). In addition, several selected compds. were evaluated as substrates for T. gondii UPRTase, and it was found that 2,4-dithiouracil is also a substrate for this enzyme. On the basis of these data, a structure-activity relationship for the binding of ligands to T. gondii UPRTase was determined using uracil as a reference compound
IT **17687-24-0**, 5-Nitroorotic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(as ligand of uracil phosphoribosyltransferase from Toxoplasma gondii, structure in relation to)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 39 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:124131 CAPLUS
DN 120:124131
TI Structure-activity relationship of nucleobase ligands of uridine phosphorylase from Toxoplasma gondii
AU Iltzsch, Max H.; Klenk, Elizabeth E.
CS Dep. Biol. Sci., Univ. Cincinnati, Cincinnati, OH, 45221-0006, USA
SO Biochemical Pharmacology (1993), 46(10), 1849-58
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB Seventy-nine nucleobase analogs were evaluated as potential inhibitors of T. gondii uridine phosphorylase (UrdPase), and the apparent Ki (appKi) values for these compds. were determined Based on the inhibition data, a structure-activity relationship for the binding of nucleobase analogs to the enzyme was formulated, using uracil as a reference compound Two compds. were identified as very potent inhibitors of T. gondii UrdPase: 5-benzyloxybenzylbarbituric acid and 5-benzyloxybenzyluracil, which had appKi values of 0.32 and 2.5 μM, resp. A comparison of the results from the present study with those from similar studies on mammalian UrdPase and thymidine phosphorylase (dThdPase) revealed that there are both similarities and differences between the catalytic site of T. gondii UrdPase and the catalytic sites of the mammalian enzymes with respect to binding of uracil analogs. One compound, 6-benzyl-2-thiouracil, was identified as a potent, specific inhibitor (appKi = 14 μM) of T. gondii UrdPase, relative to mammalian UrdPase and dThdPase.
IT **17687-24-0,** 5-Nitroorotic acid
RL: BIOL (Biological study)
(uridine phosphorylase of Toxoplasma gondii inhibition by, structure in relation to)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

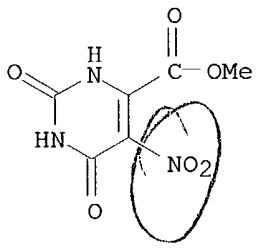


L6 ANSWER 40 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:517246 CAPLUS
DN 119:117246
TI Preparation and formulation of fused heterocyclic compounds as angiotensin II antagonists
IN Naka, Takehiko; Inada, Yoshiyuki
PA Takeda Chemical Industries, Ltd., Japan
SO Can. Pat. Appl., 160 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

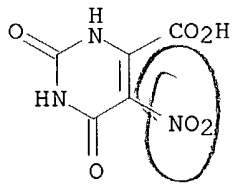
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2066094	AA	19921017	CA 1992-2066094	19920415
	CA 2066094	C	20030624		
	JP 05163267	A2	19930629	JP 1992-137485	19920415
	JP 3260415	B2	20020225		
	JP 2001328988	A2	20011127	JP 2001-159745	19920415
	EP 518033	A1	19921216	EP 1992-106621	19920416
	EP 518033	B1	20030702		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE				
	AT 244240	E	20030715	AT 1992-106621	19920416
	EP 1327631	A2	20030716	EP 2003-6453	19920416
	EP 1327631	A3	20040211		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT				
	US 5389641	A	19950214	US 1993-127356	19930928
PRAI	JP 1991-173473	A	19910416		
	JP 1991-263341	A	19910705		
	JP 1991-315629	A	19910925		
	JP 1992-137485	A3	19920415		
	EP 1992-106621	A3	19920416		
	US 1992-868841	B1	19920416		

OS MARPAT 119:117246
AB Title compds. (I R1 = an optionally substituted hydrocarbon residue which may be attached through a hetero atom; R2 = a group capable of forming an anion or a group convertible thereinto; R3 = an optionally substituted aromatic hydrocarbon or heterocyclic residue which contains at least one hetero atom; X = a direct bond or a spacer having an atomic length of two or less between the R3 group and the ring W group; W = an optionally substituted aromatic hydrocarbon or heterocyclic residue which contains at least one hetero atom; a, c and d are independently selected from the group consisting of one or two optionally substituted carbon atoms and one or two optionally substituted hetero atoms; b and e are independently selected from the group consisting of one optionally substituted carbon atom and one optionally substituted nitrogen atom; the dotted line is a bond to form one double bond; n is an integer of 1 or 2 and when a, which is an optionally substituted carbon atom, is taken together with R1, R1c:a may form a ring) were prepared Thus, 3-methyl-4,5-diaminopyridine was cyclocondensed with BuCO2H and the product converted in 3 steps to imidazopyridinecarboxylate II (R = H, R4 = Me) which was condensed with R5Br (R5 = biphenylylmethyl group Q, R6 = CPh3) to give, after deprotection and saponification, II (R = Q, R4 = R6 = H) which gave 63% inhibition of angiotensin II binding at 10-7M in vitro.
IT **6311-73-5P 17687-24-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

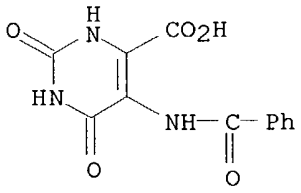
(preparation and reaction of, in preparation of angiotensin II inhibitors)
RN 6311-73-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

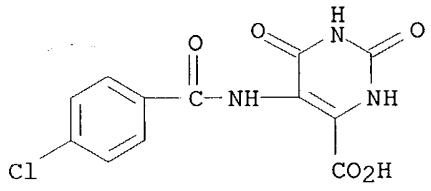


L6 ANSWER 41 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:116216 CAPLUS
DN 118:116216
TI Synthesis and pharmacological properties of 2,4-disubstituted 5-amino-6-pyrimidinecarboxylic acid derivatives. Part II
AU Jasztold-Howorko, Ryszard; Machon, Zdzislaw; Wilimowski, Marian; Wojewodzki, Wieslaw; Barczynska, Jadwiga; Kedzierska, Lidia; Orzechowska-Juzwenko, Krystyna; Dus, Ewa; Rutkowska, Maria; Szelag, Adam
CS Dep. Org. Chem., Med. Acad., Wroclaw, 50-137, Pol.
SO Polish Journal of Pharmacology and Pharmacy (1992), 44(4), 393-406
CODEN: PJPPAA; ISSN: 0301-0244
DT Journal
LA English
AB 2,4-Disubstituted 5-amino-6-pyrimidinecarboxylic acid derivs. (I; R = H or Cl; R1 = alkyl- or arylamino) were synthesized and evaluated for their pharmacol. activity on the central nervous system. Some compds. had an antiaggressive effect, others displayed antiserotonin activity, while 1 compound exerted antireserpine action. Structure-activity relations are discussed.
IT **59662-86-1 82241-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 59662-86-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

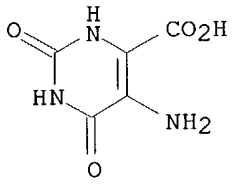


Same as #71

RN 82241-27-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorobenzoyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

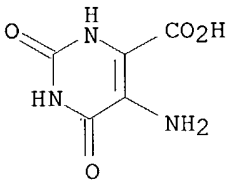


L6 ANSWER 42 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:230659 CAPLUS
DN 116:230659
TI The mechanism of action and mode of inhibition of dihydroorotate dehydrogenase. A quantum chemical study
AU Mahmoudian, M.; Pakiari, A. H.; Khademi, S.
CS Dep. Pharmacol., Univ. Med. Sci. Iran, Tehran, 15934, Iran
SO Biochemical Pharmacology (1992), 43(2), 283-7
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB Semi-empirical quantum chemical calcns. were applied to study the reaction mechanism and mode of inhibition of dihydroorotate dehydrogenase (I). The structure of substrate, intermediate, product and various inhibitors of I were optimized using the MNDO method and the geometry, heat of formation, and the net atomic partial charges of optimized mols., as well as the energy of the reaction path were calculated This study showed that the carbanion intermediate of this reaction is rather stable (heat of formation = -134.5 kcal) and readily forms upon nucleophilic attack by groups such as the hydroxyl ion. There was a good correlation between the electronic properties and the biol. activities of various inhibitors of I; the geometry of the most active inhibitor resembled closely that of the reaction intermediate. It was concluded that the oxidation by I proceeds via formation of an intermediate and that the inhibitors bind to the active site of this enzyme in the place of this intermediate.
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase inhibition by, quantum chemical study of, inhibitor structure in relation to)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as 25

L6 ANSWER 43 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:227682 CAPLUS
DN 116:227682
TI Antimalarial activity of orotate analogs that inhibit dihydroorotase and dihydroorotate dehydrogenase
AU Krungkrai, Jerapan; Krungkrai, Sudaratana R.; Phakanont, Kritsana
CS Fac. Med., Chulalongkorn Univ., Bangkok, 10330, Thailand
SO Biochemical Pharmacology (1992), 43(6), 1295-301
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB Dihydroorotase and dihydroorotate dehydrogenase, two enzymes of the pyrimidine biosynthetic pathway, were purified from Plasmodium berghei to apparent homogeneity. Orotate and a series of 5-substituted derivs. were found to inhibit competitively the purified enzymes from the malaria parasite. The order of effectiveness as inhibitors on pyrimidine ring cleavage reaction for dihydroorotase was 5-fluoroorotate > 5-aminoorotate, 5-Me-orotate > orotate > 5-bromoorotate > 5-iodoorotate with Ki values of 65, 142, 166, 860, 2200 and >3500 μM, resp. 5-Fluor orotate and orotate were the most effective inhibitors for dihydroorotate dehydrogenase. In vitro, 5-fluoroorotate and 5-aminoorotate caused 50% inhibition of the growth of P. falciparum at concns. of 10 nM and 1 μM, resp. In mice infected with P. berghei, these two orotate analogs at a dose of 25 mg/kg body weight eliminated parasitemia after a 4-day treatment, an effect comparable to that of the same dose of chloroquine. The infected mice treated with 5-fluoroorotate at a lower dose of 2.5 mg/kg had a 95% reduction in parasitemia. The effects of the more potent compds. tested in combination with inhibitors of other enzymes of this pathway on P. falciparum in vitro and P. berghei in vivo are currently under investigation. These results suggest that the pyrimidine biosynthetic pathway in the malarial parasite may be a target for the design of antimalarial drugs.
IT **7164-43-4**
RL: BIOL (Biological study)
(antimalarial activity and dihydroorotase and dihydroorotate dehydrogenase of, structure in relation to)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

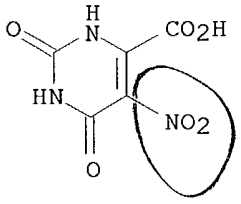
L6 ANSWER 44 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:648073 CAPLUS
DN 115:248073
TI Antimalarial compositions containing pyrimidine analog inhibitors of nucleic acid biosynthesis
IN Rathod, Pradipsinh K.
PA Catholic University of America, USA
SO PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9100081	A2	19910110	WO 1990-US3271	19900614
	WO 9100081	A3	19911212		
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	EP 445239	A1	19910911	EP 1990-909947	19900614
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
	JP 04503814	T2	19920709	JP 1990-509867	19900614
	US 6159953	A	20001212	US 1992-851103	19920316
PRAI	US 1989-369472	A	19890621		
	WO 1990-US3271	W	19900614		

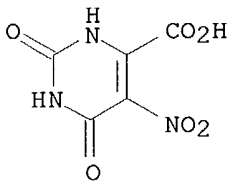
AB Antimalarial compns. comprise ≥1 pyrimidine derivs. as nucleic acid biosynthesis inhibitors in malaria parasites, alone or together with ≥1 pyrimidine base or nucleoside that can be used by a subject infected with malaria parasites, but not by parasites themselves, to synthesize nucleic acids. The composition can be formulated for oral or parenteral administration. A potent antimalarial activity of 5-fluoroorotic acid (I) against Plasmodium falciparum in vitro was demonstrated. Mice infected by i.p. injection of erythrocytic forms of P. yoelii received 0.2-5 mg I/kg plus 800 mg uridine/kg in saline solution; I exhibited a dose-dependent ability to suppress parasitemia in mice.

IT **17687-24-0**, 5-Nitroorotic acid **17687-24-0D**,
5-Nitroorotic acid, derivs.
RL: BIOL (Biological study)
(malaria treatment with)

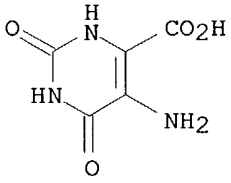
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



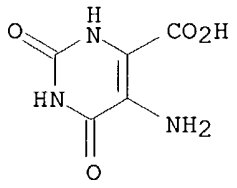
L6 ANSWER 46 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:94091 CAPLUS
DN 114:94091
TI Synthesis, physical properties and spectroscopic studies of isoorotato, 5-aminoorotato and 2-thiooratato lanthanide(III) complexes
AU Perlepes, S. P.; Lazaridou, V.; Sankhla, B.; Tsangaris, J. M.
CS Dep. Chem., Univ. Ioannina, Ioannina, 45110, Greece
SO Bulletin de la Societe Chimique de France (1990), (Sept.-Oct.), 597-608
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA English
AB Ln(H2L3·nH2O (H3L = isoorotic acid (H3isor), 5-aminoorotic acid (H3amor), 2-thioorotic acid (H3thor); Ln = lanthanides were isolated. The complexes were characterized by elemental analyses, conductivity measurements, thermal (TG, DTG, DTA) methods, x-ray powder patterns, magnetic moments, and spectral (IR, 1H NMR, electronic diffuse reflectance and emission f-f spectra) studies. All the data are discussed in terms of the nature of the bonding and the possible structural types. The neutral secondary amide and thioamide groups and the amino N-atom of H2amor- and H2thor- coordinated to the metal ions. The carboxylate group exhibits bidentate coordination in the polymeric H2amor- and H2thor- complexes, while H2isor- behaves as a bidentate ocarboxylate, O(4) ligand giving monomeric complexes. The anhydrous species obtained by thermal decomposition of the initially isolated complexes were studied.
IT **132098-29-4P 132098-30-7P 132098-44-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 132098-29-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, thulium(3+) salt (3:1) (9CI) (CA INDEX NAME)



Same as #25

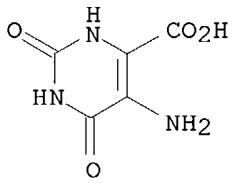
●1/3 Tm(III)

RN 132098-30-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, ytterbium(3+) salt (3:1) (9CI) (CA INDEX NAME)



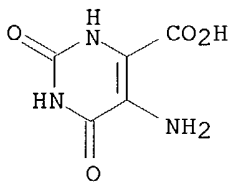
● 1/3 Yb(III)

RN 132098-44-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, monosodium salt (9CI) (CA INDEX NAME)



● Na

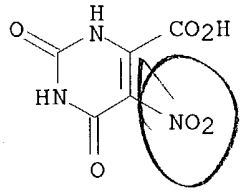
IT **7164-43-4**, 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium hydroxide)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 47 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:84878 CAPLUS
DN 114:84878
TI Gas generant compositions containing salts of 5-nitrobarbituric acid, salts of nitroorotic acid, or 5-nitrouracil
IN Wardle, Robert B.; Edwards, W. Wayne
PA Morton International, Inc., USA
SO Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 400809	A2	19901205	EP 1990-304498	19900426
	EP 400809	A3	19911016		
	EP 400809	B1	19940316		
	R: DE, ES, FR, GB, IT, SE				
	US 5015309	A	19910514	US 1989-347540	19890504
	CA 2013016	AA	19901104	CA 1990-2013016	19900326
	CA 2013016	C	19931130		
	AU 9052279	A1	19901108	AU 1990-52279	19900327
	AU 620703	B2	19920220		
	JP 02302388	A2	19901214	JP 1990-100533	19900418
	JP 06076272	B4	19940928		
	ES 2053106	T3	19940716	ES 1990-304498	19900426
PRAI	US 1989-347540		19890504		

OS MARPAT 114:84878
AB The title compns. comprise a heterocyclic compound having the structure I wherein R is H, CO2X or OX and X being a cation selected from metals of Group IA (except Na), Ca, Sr, or Ba such as a salt of 5-nitrobarbituric acid 25-75, an anhydrous oxidizing salt having a cation selected from metals of Group IA (except Na), Ca, Sr, or Ba and an anion which is free of C, H, or halogens such as KNO3 25-75, and a binder such as polypropylene carbonate or MoS2 <5 weight%. The composition is burned to provide inflation for automobile airbag restraint systems.
IT **60779-49-9**
RL: USES (Uses)
(gas generant containing, for airbag)
RN 60779-49-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, potassium salt (9CI) (CA INDEX NAME)



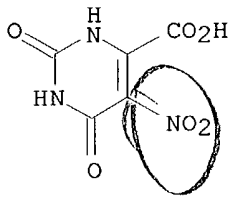
●x K

L6 ANSWER 48 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:42810 CAPLUS
DN 114:42810
TI Preparation of 5-aminoorotic acid
IN Gaset, Antoine; Delmas, Michel; Godawa, Christine; Rostiaux, Muriele; Raysse, Georges
PA Societe Nationale des Poudres et Explosifs, Fr.
SO Fr. Demande, 10 pp.
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

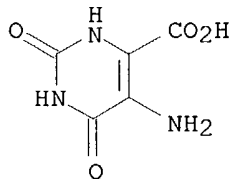
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2640265	A1	19900615	FR 1988-16434	19881214
	FR 2640265	B1	19910719		
PRAI	FR 1988-16434		19881214		

AB The title compound is prepared by hydrogenation of 5-nitroortic acid as its alkaline salts in an aqueous alc. solution comprising 15-30 volume% EtOH or MeOH (or a mixture of these) containing KOH in the presence of a Pd catalyst at 30-70° under 2-4 MPa H.

IT **17687-24-0**, 5-Nitroorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, aminoorotic acid from, method for)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

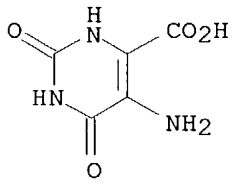


IT **7164-43-4P**, 5-Aminoorotic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by hydrogenation of nitroorotic acid, method for)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



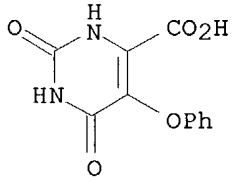
Same as #25

L6 ANSWER 49 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:6134 CAPLUS
DN 114:6134
TI Investigation of azoles and azines. 76. Mass spectra of 5- and 6-substituted uracils
AU Mirzoyan, V. S.; Melik-Ogandzhanyan, R. G.; Rusavskaya, T. N.; Studentsov, E. P.; Ivin, B. A.
CS Leningr. Khim.-Farm. Inst., Leningrad, 197022, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1990), (4), 520-31
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
AB Mass spectra of 39 substituted uracils I (R1, R3 = H, Me, R5 = NO2, halo, amino, H, CO2H, R6 = H, Cl, F, MeO, amino, CO2H) were determined
IT **7164-43-4 14383-34-7 17687-24-0**
RL: PRP (Properties)
(mass spectra of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

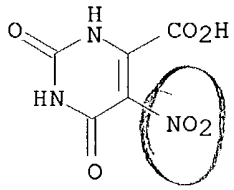


RN 14383-34-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-phenoxy- (9CI) (CA INDEX NAME)

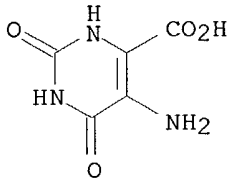
Same as #39



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

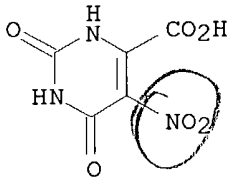


L6 ANSWER 50 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:419878 CAPLUS
DN 113:19878
TI Pyrimidine biosynthesis in parasitic protozoa: purification of a monofunctional dihydroorotase from Plasmodium berghei and Crithidia fasciculata
AU Krungkrai, Jerapan; Cerami, Anthony; Henderson, Graeme B.
CS Lab. Med. Biochem., Rockefeller Univ., New York, NY, 10021, USA
SO Biochemistry (1990), 29(26), 6270-5
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB Dihydroorotase (DHOase) was purified from 2 parasitic protozoa, C. fasciculata (.apprx.16,000-fold) and P. berghei (.apprx.790-fold). The C. fasciculata enzyme had a native mol. weight (Mr) of 42,000, determined by gel filtration chromatog., and showed a single detectable protein band on SDS-PAGE with a Mr of 44,000. The DHOase from P. berghei had a native Mr of 40,000 and a subunit Mr on SDS-PAGE of 38,000. The DHOase from both parasites, in contrast to the mammalian enzyme which residues on a trifunctional protein of the 1st 2 enzymes of the pyrimidine biosynthesis pathway, carbamoylphosphate synthase and aspartate transcarbamylase, is a monomeric enzyme and has no oligomeric structure as studied by chemical crosslinking with di-Me suberimidate. The rate of cyclization of N-carbamoyl-L-aspartate (L-CA) by the C. fasciculata enzyme was relatively high at acidic pH, decreasing to a very low rate at alkaline pH. In contrast, the rate of ring cleavage of L-5,6-dihydroorotate (L-DHO) was very low at acidic pH and increased to higher rate at alkaline pH. These pH-activity profiles gave an intersection at pH 6.6. The Km and kcat for L-CA were 0.846 mM and 39.2 min-1, resp.; for L-DHO, they were 25.85 μM and 258.6 min-1. The cryoprotectant DMSO used as stabilizing agent in the complete purification and storage, markedly affected the DHOase activity. DMSO increased the catalytic efficiency of the enzyme, as measured by kcat/Km, in the ring cyclization reaction but had no effect on the ring cleavage reaction. In spite of their marked phys. differences, kinetic and inhibitor studies with 5-substituted derivs. of orotic acid suggest that the protozoan, mammalian, and prokaryotic enzymes have a common catalytic mechanism.
IT **7164-43-4**, 5-Aminoorotic acid
RL: BIOL (Biological study)
(dihydroorotase of Plasmodium berghei inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

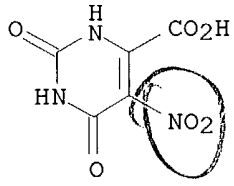


Same as #25

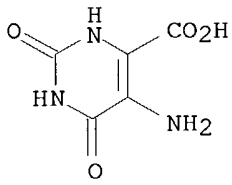
L6 ANSWER 51 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:228806 CAPLUS
DN 112:228806
TI Electroanalytical study of the anodic wave of 5-nitroorotic acid
AU Rodriguez Flores, J.; Calvo Blazquez, L.; Marin Sanchez, C.; Sanchez Misiego, A.
CS Dep. Anal. Chem. Electrochem., Univ. Extremadura, Badajoz, Spain
SO Proceedings - Indian Academy of Sciences, Chemical Sciences (1990), 102(1), 25-9
CODEN: PIAADM; ISSN: 0253-4134
DT Journal
LA English
AB The electroanal. behavior of 5-nitroorotic acid was studied at several pH values, using d.c. and differential pulse polarog. and cyclic voltammetry techniques. 5-Nitroorotic acid undergoes one oxidation wave in the pH interval considered, due oxidation of Hg and complexation of Hg(II) with 5-nitroorotic acid. The best conditions for determination of Hg(II) in the presence of the acid were also studied.
IT **17687-24-0**, 5-Nitroorotic acid
RL: ANST (Analytical study)
(anodic polarog. and voltammetric waves and use of, in amperometric determination of mercury)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **17687-24-0D**, 5-Nitroorotic acid, mercury complex
RL: PROC (Process)
(polarog. and cyclic voltammetry of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

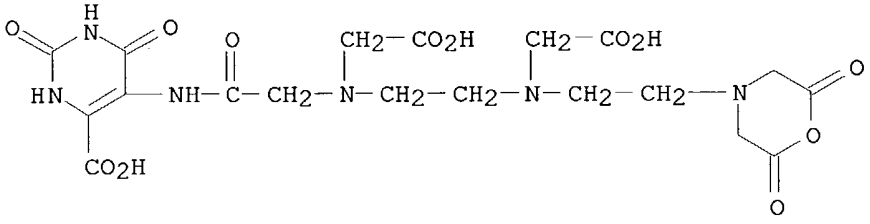


L6 ANSWER 52 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:195107 CAPLUS
DN 112:195107
TI Inhibition of uridine phosphorylase from Giardia lamblia by pyrimidine analogs
AU Jimenez, Barbara M.; Kranz, Peter; Lee, Choy Soong; Gero, Annette M.; O'Sullivan, William J.
CS Sch. Biochem., Univ. New South Wales, Kensington, 2033, Australia
SO Biochemical Pharmacology (1989), 38(21), 3785-9
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB Fifty-six pyrimidine analogs were tested as possible inhibitors of uridine phosphorylase from G. lamblia. Values of Ki were determined for eight of these which demonstrated an inhibition >60% under the standard conditions of uridine at 1 mM (approx. 1.5 times the Km) and inhibitor at 1 mM. All were competitive with respect to uridine. The most effective inhibitors were uracil analogs substituted at the C-5 position with electron-withdrawing groups (nitro groups or halogens). The inhibitory effect at the 5-position appeared to be further enhanced by substitution at the C-6 position with electron-releasing groups. The order of effectiveness as inhibitors was 6-methyl-5-nitrouracil > 6-amino-5-nitrouracil > 5-benzylacyclouridine > 5-nitrouracil > 5-fluorouracil > 5-bromouracil > 6-benzyl-2-thiouracil > 1,3-dimethyluracil, with Ki values of 10, 12, 44, 56, 119, 230, 190 and >1000 μM, resp. The compds. were also effective inhibitors of the thymidine phosphorylase activity of the enzyme. The results are discussed in relation to the use of these pyrimidine analogs to treat G. lamblia infections.
IT **7164-43-4**, 5-Aminoorotic acid
RL: BIOL (Biological study)
(uridine phosphorylase-inhibiting activity of, Giardia lamblia inhibition and structure in relation to)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

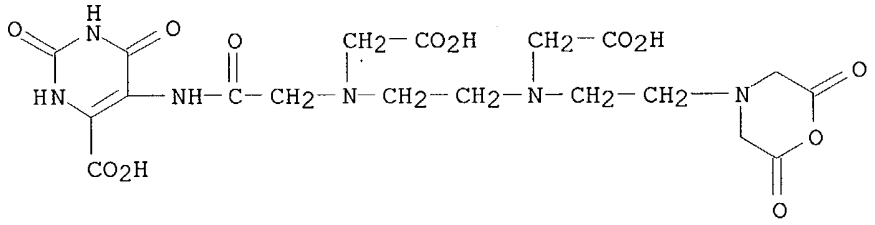


Same as #23

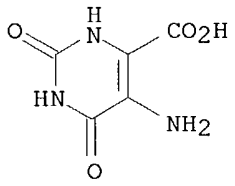
L6 ANSWER 53 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:115231 CAPLUS
DN 112:115231
TI Fluorescent terbium chelates derived from diethylenetriaminepentaacetic acid and heterocyclic compounds
AU Canfi, Ayala; Bailey, M. Philip; Rocks, Bernard F.
CS Biochem. Dep., R. Sussex County Hosp., Brighton/Sussex, BN2 5BE, UK
SO Analyst (Cambridge, United Kingdom) (1989), 114(11), 1405-6
CODEN: ANALAO; ISSN: 0003-2654
DT Journal
LA English
AB A series of aminoarom. derivs. of diethylenetriaminepentaacetic acid (DTPA) was prepared, in a search for terbium chelates suitable for use in fluorescence immunoassay. Most of the derivs. contained heterocyclic rings with at least 1 nitrogen atom. The fluorescence properties of the terbium chelate of each compound were examined Although none of the products proved suitable for use in immunoassays, the terbium chelate formed from the product of the reaction between DTPA anhydride and cytosine (4-amino-2-hydroxypyrimidine) was particularly fluorescent and had a long fluorescence lifetime. It was unstable, in aqueous solution below pH 9. The fluorescence properties of some europium complexes were also examined
IT **125502-84-3DP,** europium and terbium complexes
RL: PREP (Preparation)
(preparation and fluorescence of and stability of)
RN 125502-84-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[[[(carboxymethyl)[2-[(carboxymethyl)[2-(2,6-dioxo-4-morpholinyl)ethyl]amino]ethyl]amino]acetyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



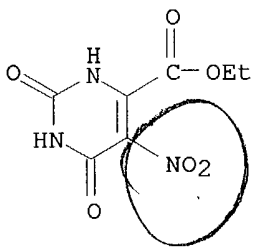
IT **125502-84-3P**
RL: PREP (Preparation)
(preparation of)
RN 125502-84-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[[[(carboxymethyl)[2-[(carboxymethyl)[2-(2,6-dioxo-4-morpholinyl)ethyl]amino]ethyl]amino]acetyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethylenetriaminepentaacetic acid anhydride)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 54 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:55445 CAPLUS
DN 112:55445
TI New derivatives of 5-nitroorotic acid, and the synthesis of 4-ethoxycarbonyl-2-(N-methylanilino)-5,6,7,8-tetrahydropteridine
AU Boyle, Peter H.; Gillespie, Paul
CS Univ. Chem. Lab., Trinity Coll., Dublin, Ire.
SO Journal of Chemical Research, Synopses (1989), (9), 282
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
OS CASREACT 112:55445
AB In the search for a model tetrahydropteridine which would be stable in air and soluble in organic solvents, the title compound (I) was prepared which was found to fit both of these criteria. In the course of the synthesis, a series of new pyrimidine derivs. was prepared and characterized.
IT **52047-16-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)
RN 52047-16-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



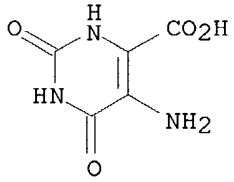
L6 ANSWER 55 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:478025 CAPLUS
DN 111:78025
TI Preparation of 2,4,6,8-tetrahydroxypyrimido[5,4-d]pyrimidine, an intermediate for cardiovascular agents, from 5-aminouracil-4-carboxylic acid and urea
IN Niegel, Harald; Meyer, Hans Peter; Lorenz, Dieter; Born, Michael; Nauwald, Gunter
PA VEB Arzneimittelwerk, Ger. Dem. Rep.
SO Ger. (East), 4 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DD 263891	A3	19890118	DD 1986-298275	19861223
PRAI	DD 1986-298275		19861223		

AB The title compound (I), useful as an intermediate for cardiovascular agents, was prepared by cyclocondensation of 5-aminouracil-4-carboxylic acid (II) with urea in the presence of Et3N+CH2Ph Cl- (III) and a polyether alc. at 140-190° for 3-6 h followed by treatment with H2O at 100°. A mixture of II, III, and urea was mixed in a preheated (80-100°) reactor. A polyether alc. with average mol. weight 1000-2000 was added and the mixture was heated at 150-170° for 6 h. H2O and then aqueous NaOH was added at 100° to give 87% I.2Na of 98% purity.

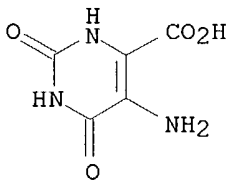
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with urea)

RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

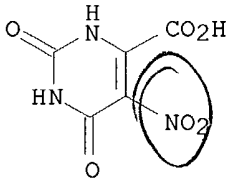


Same as #25

L6 ANSWER 56 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:433117 CAPLUS
DN 111:33117
TI Structure-activity relationship of ligands of dihydrouracil dehydrogenase from mouse liver
AU Naguib, Fardos N. M.; El Kouni, Mahmoud H.; Cha, Sungman
CS Div. Biol. Med., Brown Univ., Providence, RI, 02912, USA
SO Biochemical Pharmacology (1989), 38(9), 1471-80
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB One hundred and five nucleobase analogs were screened as inhibitors of dihydrouracil dehydrogenase (DHUDase, EC 1.3.1.2) from mouse liver. 5-Benzyloxybenzyluracil, 1-deazauracil (2,6-pyridinediol), 3-deazauracil (2,4-pyridinediol), 5-benzyluracil, 5-nitrobarbituric acid and 5,6-dioxyuracil (alloxan) were identified as potent inhibitors of this activity, with apparent Ki values of 0.2, 0.5, 2.1, 3.4, 3.8 and 6.6 μM resp. Both 5-benzyloxybenzyluracil and 1-deazauracil were also potent inhibitors of DHUDase from human livers. These findings along with an extensive review of literature allowed the formulation of a structure-activity relationship. The binding to DHUDase required intact C2 and C4 oxo groups. Replacement of N1 or N3 by an endocyclic carbon enhanced binding. In contrast, replacement of C5 or C6 by an endocyclic nitrogen abolished binding. Addition of a charged group to C5 and/or C6, and of a hydrophobic group to C5 but not C6 improved the binding.
IT **7164-43-4**, 5-Aminoorotic acid **17687-24-0**, 5-Nitroorotic acid
RL: BIOL (Biological study)
(dihydrouracil dehydrogenase inhibition by, from liver, structure in relation to)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



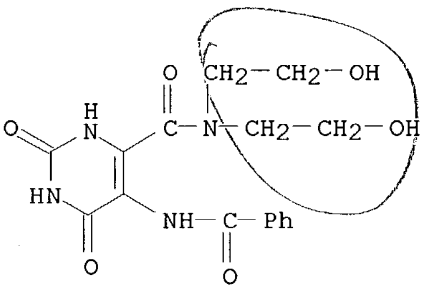
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



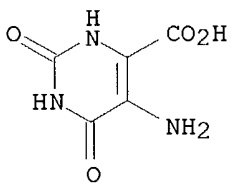
L6 ANSWER 57 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:114862 CAPLUS
DN 110:114862
TI Process for preparing 2-(β-isopropylaminoethyl)-8-hydroxy-9-(benzoylamino)perhydropyrazino[1,2-c]pyrimidine-1-,6-dione affecting central nervous system
IN Machon, Zdzislaw; Jasztold-Howorko, Ryszard; Wilimowski, Marian
PA Akademia Medyczna, Wroclaw, Pol.
SO Pol., 3 pp.
CODEN: POXXA7
DT Patent
LA Polish
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PL 129506	B2	19840531	PL 1982-238393	19820928
PRAI PL 1982-238393		19820928		

OS CASREACT 110:114862
AB The title compound (I) is prepared from 1-benzoyl-2-oxo-4,6-dihydroxyazetino[3,2-d]pyrimidine. The latter is reacted with diethanolamine in an anhydrous alc. to give 2,4-dihydroxy-5-benzoylamino-6-pyrimidinocarboxylic acid diethanolamide (yield 85%) which is reacted with thionyl chloride in anhydrous benzene to give 2-β-chloroethyl-8-hydroxy-9-benzoylaminoperhydropyrazino[1,2-c]pyrimidine-1,6-dione (yield 50%). The latter is reacted with isopropylamine at room temperature to obtain I (yield 50%). In animal tests, I affects the central nervous system. I has lower toxicity than that of conventional depressants. I has an LD50 of 0.4 at a dose of 16.68 mg/kg, compared to 0.077 LD50 for 10 mg imipramine/kg.
IT **103720-96-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and chlorination-cyclization of, pyrazinopyrimidine derivative from)
RN 103720-96-3 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-1,2,3,6-tetrahydro-N,N-bis(2-hydroxyethyl)-2,6-dioxo- (9CI) (CA INDEX NAME)

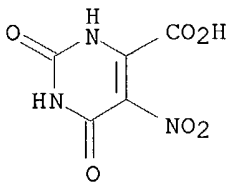


L6 ANSWER 58 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:71668 CAPLUS
DN 110:71668
TI Structure-activity relationships of pyrimidines as dihydroorotate dehydrogenase inhibitors
AU DeFrees, Shawn A.; Sawick, David P.; Cunningham, Brady; Heinstein, Peter F.; Morre, D. James; Cassady, John M.
CS Sch. Pharm. Pharmacal Sci., Purdue Univ., West Lafayette, IN, 47907, USA
SO Biochemical Pharmacology (1988), 37(20), 3807-16
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB This paper reports results on a series of pyrimidine analogs of dihydroorotate (DHO) and orotic acid (OA) as inhibitors of DHO-dehase (dihydroorotate dehydrogenase). The enzyme test results established that the intact amide and imide groups of the pyrimidine ring and the 6-carboxylic acid are required for significant enzyme inhibition. The testing of several functional groups similar in characteristics to that of the carboxylic acid, such as sulfonamide, tetrazole, and phosphate, indicated that the carboxylic acid group is preferred by the enzyme. Using various 5-substituted OA and DHO derivs., it was shown that there is a steric limitation of a Me group at this position. The compound DL-5-trans-Me DHO (Ki of 45 μM) was both an inhibitor and a weak substrate for the enzyme, demonstrating that mechanism-based enzyme inhibitors should be effective. The testing results further suggest that a neg. charged enzyme substituent may be present near the 5-position of the pyrimidine ring and that there may be an enzyme-substrate metal coordination site near the N-1 and carboxylic acid positions of the pyrimidine ring. The combined testing results were then used to define both conformational and steric substrate-enzyme binding requirements from which a model was proposed for the binding of DHO and OA to the DHO-dehase active site.
IT **7164-43-4 17687-24-0**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase of liver mitochondria inhibition by, structure-activity relationships in relation to)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

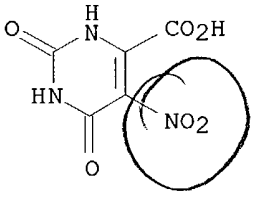


Search AD #25

RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 59 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:629962 CAPLUS
DN 109:229962
TI Electroanalytical behavior of 5-nitroorotic acid
AU Rodriguez, J.; Calvo, L.; Marin, C.; Sanchez, A.
CS Dep. Anal. Chem. Electrochem., Univ. Extremadura, Badajoz, Spain
SO Proceedings - Indian Academy of Sciences, Chemical Sciences (1988), 100(1), 27-9
CODEN: PIAADM; ISSN: 0253-4134
DT Journal
LA English
AB The electroanal. behavior of 5-nitroorotic acid (I) was studied at several pH values, using several techniques (DC and DP polarog. and CV). I undergoes five irreversible diffusion-controlled reduction waves over the pH range considered. The optimum conditions for determination of I are also studied.
IT **17687-24-0,** 5-Nitroorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(electrochem. reduction of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

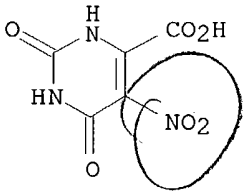


L6 ANSWER 60 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:56118 CAPLUS
DN 108:56118
TI A process for preparation of 5-aminoorotic acid
IN Morbidelli, Giuseppe; Amori, Dario
PA Recordati S. A. Chemical and Pharmaceutical Co., Switz.
SO Fr. Demande, 4 pp.
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

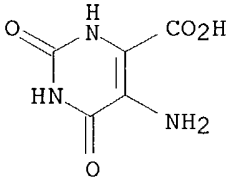
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2589153	A1	19870430	FR 1985-15902	19851025
	FR 2589153	B1	19880923		
PRAI	FR 1985-15902		19851025		

AB The title compound (I), useful as an intermediate for dipyridamole, is prepared by reduction of of 5-nitroorotic acid (II). K 5-nitroorotate.H2O and an aqueous suspension of Raney Ni were added to aqueous KOH at 20°, H (2 bars) was passed into the reaction mixture, and the resulting mixture was heated at 35-40° for .apprx.6-10 h to give 90.8% I.

IT **17687-24-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenolysis of, aminoorotic acid by)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



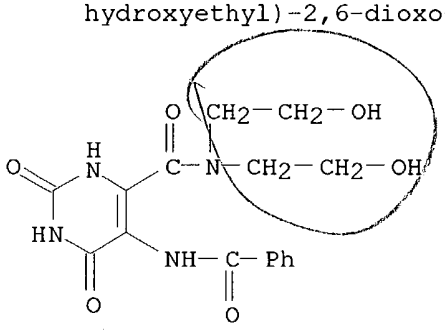
IT **7164-43-4P**, 5-Aminoorotic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by hydrogenolysis of nitroorotic acid)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 61 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:636732 CAPLUS
DN 107:236732
TI Preparation of 9-(benzoylamino)-2-(2-chloroethyl)-3,4-dihydro-8-hydroxy-2H-pyrazino[1,2-c]pyrimidine-2,6-dione
IN Machon, Zdzislaw; Josztold-Howorko, Ryszard
PA Akademia Medyczna, Wroclaw, Pol.
SO Pol., 2 pp.
CODEN: POXXA7
DT Patent
LA Polish
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PL 129505	B2	19840531	PL 1982-238394	19820928
PRAI PL 1982-238394		19820928		

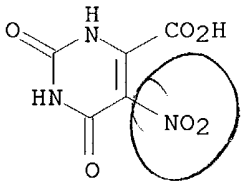
OS CASREACT 107:236732
AB The title compound (I, R = Cl) (II) was prepared in 2 steps. 1-Benzoyl-4,6-dihydroxy-2-oxoazeto[3,2-d]pyrimidine was refluxed with HN(CH2CH2OH)2 in EtOH to give 85% pyrimidinecarboxamide III which was refluxed with SOCl2 in C6H6 to give 50% II. II is an intermediate for I (R = Me2CHNH), which is a central nervous system agent that suppresses spontaneous motor activity, exhibits antiserotonin activity, and promotes the effect of DOPA (no data).
IT **103720-96-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination-cyclization of)
RN 103720-96-3 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-1,2,3,6-tetrahydro-N,N-bis(2-hydroxyethyl)-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 62 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:543703 CAPLUS
DN 107:143703
TI Alkaline baths and methods for electrodeposition of palladium and palladium alloys
IN Novel, Fred I.; Martin, James L.; Toben, Michael P.
PA Lea-Ronal, Inc., USA
SO Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 225422	A1	19870616	EP 1986-107737	19860606
	R: BE, CH, DE, FR, GB, LI, NL				
	JP 62139893	A2	19870623	JP 1986-130441	19860606
	US 4741818	A	19880503	US 1987-24874	19870317
PRAI	US 1985-808131		19851212		
	US 1985-742258		19850607		

AB The bath comprises a soluble Pd compd and ≥1 complexing agents of a corboxy-, hydroxy-, or oxo-substituted N-heterocyclic compound, e.g. chelidamic acid. For depositing Pd alloys, ≥1 soluble alloying metal compds. (e.g. Ag) can be added to the bath. The lustrous deposits can be used on elec. contacts.
IT **17687-24-0**, 5-Nitroorotic acid
RL: PRP (Properties)
(complexing agent, in baths for palladium alloy electroplating)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

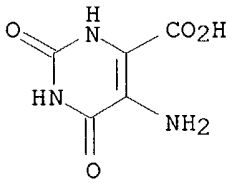


L6 ANSWER 63 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:409334 CAPLUS
DN 107:9334
TI 2,4,6,8-Tetrahydropyrimido[5,4-d]pyrimidine and its crystalline salts
IN Niegel, Harald; Meyer, Hans Peter; Lorenz, Dieter
PA VEB Arzneimittelwerk, Ger. Dem. Rep.
SO Ger. (East), 4 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 240017	A1	19861015	DD 1985-279479	19850808
PRAI DD 1985-279479		19850808		

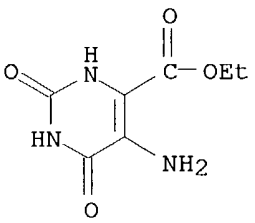
AB Crystalline 2,4,6,8-tetrahydroxypyrimido[5,4-d]pyrimidine (I) and its salts are isolated from reaction mixts. containing I, to which surfactants had been added, with stirring and colored by the addition of heated (at 80-100°) water (or aqueous acids or bases); stirring is continued to the end of crystallization and the obtained crystals separated The surfactant may be nonionic, anionic, or cationic. Suitable acids are hydrogen halides or H2SO4. 5-Amino-4-uracilcarboxylic acid (250 kg) was cyclocondensed with 800 kg urea in 50 L triethylene glycol at 160-180° for ≥8 h with stirring. The reaction mixture was cooled to 120-140°, 3 kg of ethoxylated alkylphenols (9 mols ethylene oxide) were added with stirring followed by addition of 1500-2200 L water. The suspension was stirred for 1 h at 90-100°; H2SO4 was added to adjust the pH to 1-2, and the suspension was stirred for 1 h at 90-100°, during which 212 kg I (85% theor. yield, 98% purity) precipitated, which was filtered and washed.

IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with urea)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



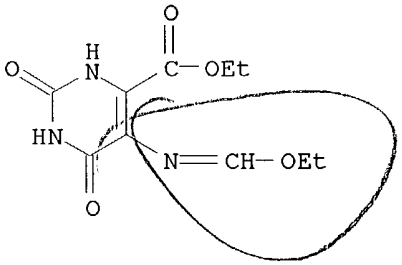
Same as #25

L6 ANSWER 64 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:213889 CAPLUS
DN 106:213889
TI Synthesis of some 7-substituted-2,4,8(1H,3H,7H)pyrimido[5,4-d]pyrimidinetriones
AU Pendergast, William; Hall, William R.
CS Wellcome Res. Lab., Research Triangle Park, NC, 27709, USA
SO Journal of Heterocyclic Chemistry (1986), 23(5), 1411-13
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 106:213889
AB The title compds. I (R = H, alkyl, cycloalkyl, benzyl, hydroxyalkyl, etc.) were prepared under mild conditions from Et 5-[(ethoxymethylene)amino]orotate (II) and RNH2. The 7-Me and 7-benzyl derivs. were methylated with tri-Me phosphate to the 1,3,7-trialkyl derivs.
IT **40598-01-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ethoxymethylenation of)
RN 40598-01-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



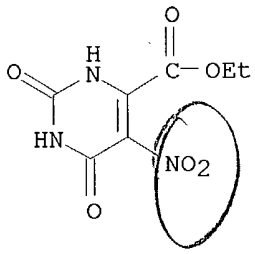
Same as #25

IT **108262-65-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with amines)
RN 108262-65-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(ethoxymethylene)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)

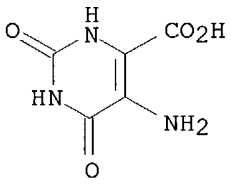


IT **52047-16-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 52047-16-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl

ester (9CI) (CA INDEX NAME)



L6 ANSWER 65 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:605173 CAPLUS
DN 105:205173
TI Affinity chromatography of cytosine deaminase from Escherichia coli with immobilized pyrimidine compounds
AU Katsuragi, Tohoru; Sakai, Takuo; Tonomura, Kenzo
CS Coll. Agric., Univ. Osaka Prefect., Osaka, 591, Japan
SO Agricultural and Biological Chemistry (1986), 50(7), 1713-19
CODEN: ABCHA6; ISSN: 0002-1369
DT Journal
LA English
AB Many classes of pyrimidine compds. were immobilized Sepharose 4B via alkyl spacers by constructing various spacers using CNBr activation of the carrier. A crude enzyme solution of E. coli with cytosine- and 5-fluorocytosine-deaminating activity was studied by adsorption and desorption chromatog. with columns of the 68 kinds of gels we made. Gels made with the following 5 ligands were effective. 2-Mercaptopyrimidine or 2-thiobarbituric acid, when coupled with 1,6-diaminohexane and then with the activated carrier, was suitable. So was 2-amino-4,6-dihydroxypyrimidine or 5-aminouracil, when linked by carbodiimide coupling to a carrier coupled with 6-aminohexanoic acid. Orotic acid, when linked in the same way with a carrier coupled with 1,4-diaminobutane, was also effective.
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with carboxypentylimino-Sepharose derivative)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

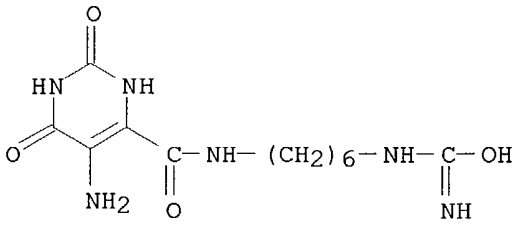


Source #25

RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with diaminohexane-Sepharose deriv.
IT **105238-19-5P 105238-21-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytosine deaminase affinity chromatog. on)
RN 105238-19-5 CAPLUS
CN Agarose, [6-[[(5-amino-1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinyl)carbonyl]amino]hexyl]carbamimidate (9CI) (CA INDEX NAME)

CM 1

CRN 172963-97-2
CMF C12 H20 N6 O4



CM 2

CRN 9012-36-6
CMF Unspecified
CCI PMS, MAN

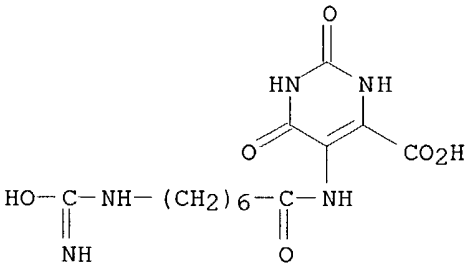
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 105238-21-9 CAPLUS

CN Agarose, [7-[(6-carboxy-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)amino]-7-oxoheptyl]carbamimidate (9CI) (CA INDEX NAME)

CM 1

CRN 173244-29-6
CMF C13 H19 N5 O6

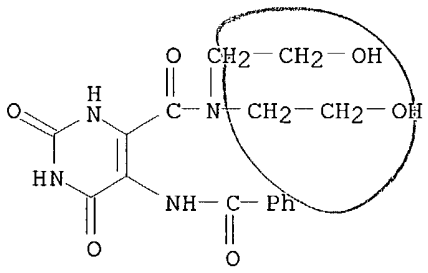


CM 2

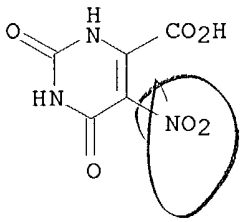
CRN 9012-36-6
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

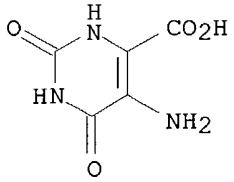
L6 ANSWER 66 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:478894 CAPLUS
DN 105:78894
TI Synthesis of perhydropyrazino[1,2-c]pyrimidine derivatives
AU Machon, Z.; Jasztold-Howorko, R.
CS Dep. Org. Chem., Med. Acad., Wroclaw, Pol.
SO Farmaco, Edizione Scientifica (1985), 40(9), 695-700
CODEN: FRPSAX; ISSN: 0430-0920
DT Journal
LA English
OS CASREACT 105:78894
AB The reaction of azetidinopyrimidine I with diethanolamine affords the amide II. Heating II with SOCl2 yields the pyrazinopyrimidinedione III (R = Cl). Reaction of III (R = Cl) with different amines gives the resp. 2-β-aminosubstituted derivs. III (R = Me2CHNH, Et2NCH2CH2NH, BuNH, PhNH, p-ClC6H4NH, morpholino, piperidino). Some of the obtained compds. showed central nervous system activity.
IT **103720-96-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of, pyrazinopyrimidine derivs. from)
RN 103720-96-3 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-1,2,3,6-tetrahydro-N,N-bis(2-hydroxyethyl)-2,6-dioxo- (9CI) (CA INDEX NAME)



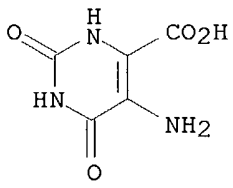
L6 ANSWER 67 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:556291 CAPLUS
DN 103:156291
TI Human spleen dihydroorotate dehydrogenase: a study of inhibition of the enzyme
AU Gero, Annette M.; O'Sullivan, William J.; Brown, Desmond
CS Sch. Biochem., Univ. New South Wales, Kensington, 2033, Australia
SO Biochemical Medicine (1985), 34(1), 60-9
CODEN: BIMDA2; ISSN: 0006-2944
DT Journal
LA English
AB Numerous pyrimidine analogs were tested as possible inhibitors of human spleen mitochondrial dihydroorotate dehydrogenase (DHO DHase). Of these, 9 were demonstrated to be effective inhibitors of the enzymic activity. Two compds., dihydro-5-azaorotate and 6-thiobarbiturate, appeared to be specific inhibitors of the DHO DHase. In addition, 3 compds., 5-azaorotate, 5-bromoorotate, and barbiturate were also inhibitory against the 2 subsequent enzymes of the pathway, orotate phosphoribosyltransferase and orotidylate decarboxylase, so that they could act against 3 enzymes of the mammalian pyrimidine de novo biosynthetic pathway.
IT **17687-24-0**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase of human spleen inhibition by)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



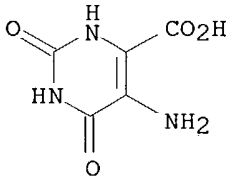
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase of human spleen inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



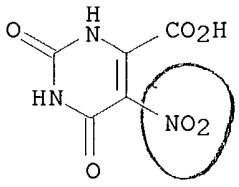
L6 ANSWER 68 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:627294 CAPLUS
DN 101:227294
TI Enzymes of uridine 5'-monophosphate biosynthesis in Schistosoma mansoni
AU Iltzsch, Max H.; Niedzwicki, John G.; Senft, Alfred W.; Cha, Sungman; El Kouni, Mahmoud H.
CS Div. Biol. Med., Brown Univ., Providence, RI, 02912, USA
SO Molecular and Biochemical Parasitology (1984), 12(2), 153-71
CODEN: MBIPDP; ISSN: 0166-6851
DT Journal
LA English
AB In S. mansoni, the major product of in vitro orotate metabolism was orotidine 5'-monophosphate (OMP), whereas in mouse liver it was UMP. In contrast to mammalian cells, OMP appeared not to be channeled from orotate phosphoriboryltransferase to OMP decarboxylase in S. mansoni, resulting in substantial degradation of OMP to orotidine. Significant differences were observed in the inhibitor specificity of phosphoribosyltransferase between S. mansoni and mouse liver, indicating that this enzyme may be a potential chemotherapeutic target in S. mansoni. Two distinct phosphoribosyltransferases were found in S. mansoni. One enzyme, having the higher mol. weight, utilized orotate, 5-fluorouracil, and uracil as substrates, whereas the other only orotate. Both enzymes were inhibited by 5-azaorotic acid (oxonic acid) but only the oratate-specific enzyme was inhibited by 4,6-dihydroxypyrimidine. OMP decarboxylase activity coeluted with both phosphoribosyltransferases from Sephadex G-100 gel chromatog. Evidently, phosphoribosyltransferase in S. mansoni plays a role in both de novo UMP biosynthesis as well as in the salvage of uracil and uridine.
IT **7164-43-4**
RL: BIOL (Biological study)
(fluorouracil reaction with phosphoribosyltransferase of schistosome inhibition by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 69 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:586788 CAPLUS
DN 101:186788
TI Structure-activity relationship of pyrimidine base analogs as ligands of orotate phosphoribosyltransferase
AU Niedzwicki, John G.; Iltzsch, Max H.; El Kouni, Mahmoud H.; Cha, Sungman
CS Div. Biol. Med., Brown Univ., Providence, RI, 02912, USA
SO Biochemical Pharmacology (1984), 33(15), 2383-95
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB Eighty pyrimidine base analogs were evaluated as inhibitors of mouse liver orotate phosphoribosyltransferase (I) (EC 2.4.2.10). Based on these findings and an extensive literature review, a structure-activity relation was formulated for the binding of pyrimidine base analogs to I. A basis for the rational design of new inhibitors of I is provided, and several such compds. are proposed. Addnl., 4,6-dihydroxypyrimidine was found to be a potent I inhibitor. Eleven I inhibitors were also evaluated as inhibitors of orotidine 5'-monophosphate decarboxylase (II) (EC 4.1.2.23). 5-Azauracil, 5-azaorotate, and barbituric acid inhibited II significantly after preincubation with PRPP and MgCl2 in the presence of cytosol.
IT **7164-43-4 17687-24-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(orotate phosphoribosyltransferase and orotidylate decarboxylase of liver cytosol inhibition by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



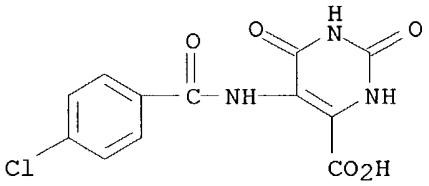
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



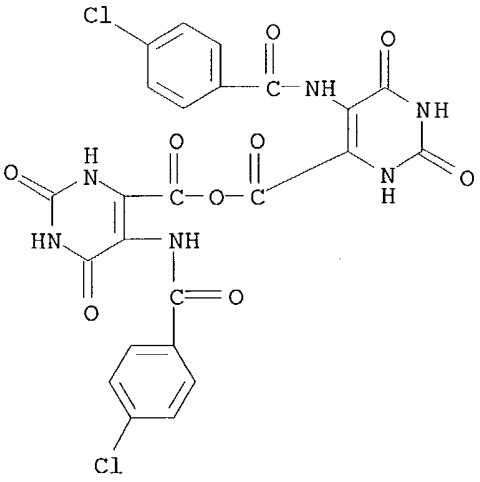
L6 ANSWER 70 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:510945 CAPLUS
DN 101:110945
TI Cyclohexylamide of 2,4-dihydroxy-5-p-chlorobenzoylaminopyrimidine-6-carboxylic acid
IN Machon, Zdzislaw; Jasztold-Howorko, Ryszard; Wilimowski, Marian
PA Akademia Medyczna, Wroclaw, Pol.
SO Pol., 4 pp.
CODEN: POXXA7
DT Patent
LA Polish
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PL 123452	B2	19821030	PL 1980-227972	19801119
PRAI PL 1980-227972		19801119		

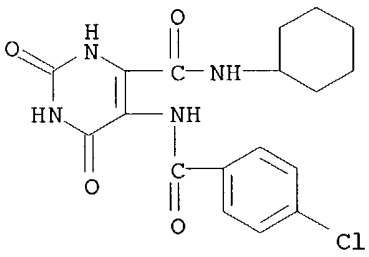
OS CASREACT 101:110945
AB The title compound (I) was prepared as, e.g., a tranquilizer (no data), by acylation of the amino acid with 4-ClC6H4COCl, then converting the acid into the cyclohexylamide via the lactam, lactone, or anhydride.
IT **82241-27-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion into cyclohexylamide)
RN 82241-27-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorobenzoyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



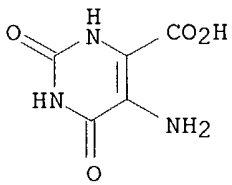
IT **91732-93-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with cyclohexylamine)
RN 91732-93-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorobenzoyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, anhydride (9CI) (CA INDEX NAME)



IT **82241-29-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82241-29-0 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-[(4-chlorobenzoyl)amino]-N-cyclohexyl-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



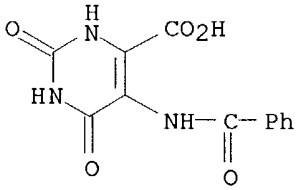
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorobenzoyl chloride)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



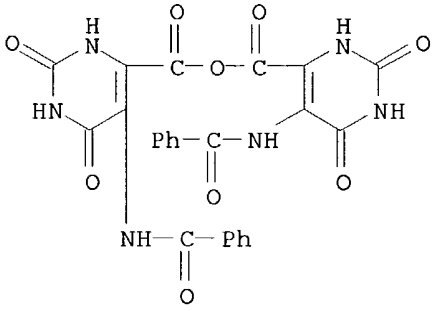
L6 ANSWER 71 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:510944 CAPLUS
DN 101:110944
TI Amide derivatives of 2,4-dihydroxy-5-(benzoylamino)pyrimidine-6-carboxylic acid
IN Machon, Zdzislaw; Jasztold-Howorko, Ryszrad; Wilimowski, Marian
PA Akademia Medyczna, Wroclaw, Pol.
SO Pol., 4 pp.
CODEN: POXXA7
DT Patent
LA Polish
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PL 122846	B2	19820831	PL 1980-227974	19801119
PRAI PL 1980-227974		19801119		

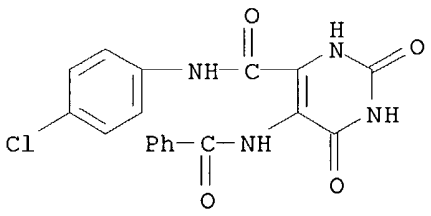
OS CASREACT 101:110944
AB Title compds. (I) (R = cyclohexyl) (II) or 4-ClC6H4) were prepared from the acid via the lactam, lactone, or anhydride, followed by reaction with, resp., cyclohexylamine or 4-ClC6H4NH2.
IT **59662-86-1**
RL: PROC (Process)
(conversion of, into amide derivs.)
RN 59662-86-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



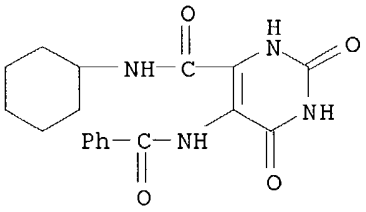
IT **91737-71-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aminolysis of)
RN 91737-71-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, anhydride (9CI) (CA INDEX NAME)



IT **82241-35-8P 82241-36-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82241-35-8 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(4-chlorophenyl)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



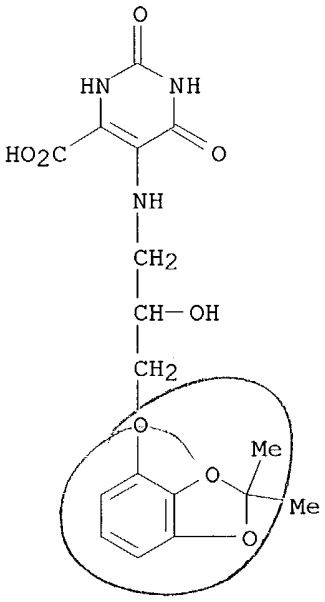
RN 82241-36-9 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-cyclohexyl-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



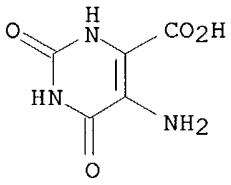
L6 ANSWER 72 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:139086 CAPLUS
DN 100:139086
TI Ring-substituted pyrogallol derivatives
IN Schlager, Ludwig H.
PA Gerot-Pharmazeutika G.m.b.H., Austria
SO Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 95454	A2	19831130	EP 1983-890068	19830502
	EP 95454	A3	19850403		
	R: BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AT 8201888	A	19840115	AT 1982-1888	19820513
	AT 375654	B	19840827		
	AT 8204671	A	19831215	AT 1982-4671	19821223
	AT 375360	B	19840725		
	AT 8301298	A	19841115	AT 1983-1298	19830412
	AT 378191	B	19850625		
	CA 1233181	A1	19880223	CA 1983-427476	19830504
	AU 8314409	A1	19831117	AU 1983-14409	19830510
	AU 566107	B2	19871008		
	DK 8302104	A	19831114	DK 1983-2104	19830511
	NO 8301680	A	19831114	NO 1983-1680	19830511
	CS 235321	B2	19850515	CS 1983-3308	19830511
	PL 141325	B1	19870731	PL 1983-241918	19830511
	JP 58206581	A2	19831201	JP 1983-81827	19830512
	DD 209831	A5	19840523	DD 1983-250870	19830512
	DD 209831	C4	19851218		
	HU 33092	O	19841029	HU 1983-1658	19830512
	CS 235344	B2	19850515	CS 1984-142	19840105
PRAI	AT 1982-1888		19820513		
	AT 1982-4671		19821223		
	AT 1983-1298		19830412		
	CS 1983-3308		19830511		

OS CASREACT 100:139086
AB 3-Benzodioxolyl ethers I [R = H, aminohydroxyalkyl, carboxyalkyl, etc.; R1, R2 = H or lower alkyl; at least one of R3-5 = halo or NO2] were prepared as analgesics and β-sympatholytics. Thus, 2,2-dimethyl-1,3-benzodioxol-4-ol was treated with epichlorohydrin, then Me3CNH2 to give the amino alc. ether II, which was superior to Atenolol as a β-blocker and a more effective analgesic than, e.g., pethidine-HCl.
IT **89085-30-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic or sympatholytic)
RN 89085-30-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[[3-[(2,2-dimethyl-1,3-benzodioxol-4-yl)oxy]-2-hydroxypropyl]amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

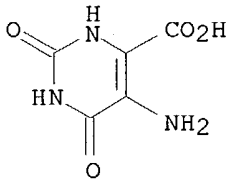

O
HN
NH
HO2C
O
NH
CH2
CH—OH
CH2
O
Me
O
Me
O

L6 ANSWER 73 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:624248 CAPLUS
DN 99:224248
TI Analytical reactions of 5-aminoorotic acid
AU Roy, B.; Singh, Ajai K.; Singh, R. P.
CS Dep. Chem., Indian Inst. Technol., Delhi, 110016, India
SO Talanta (1983), 30(8), 617-19
CODEN: TLNTA2; ISSN: 0039-9140
DT Journal
LA English
AB The potential of 5-aminoorotic acid (I) for the spectrophotometric determination of metals ions was explored. Only the reaction with Cu(II), Co(II)+, and Os(VIII) are sensitive and suitable for this purpose. Ternary complexes of Cu(II) formed with I and NH3 or pyridine can also be used for spectrophotometric determination of the metal and give better sensitivity and selectivity than the binary complex. Optimum conditions for determination of all the 3 metal ions were established.
IT **7164-43-4**
RL: ANST (Analytical study)
(in transition metal determination, spectrophotometric)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

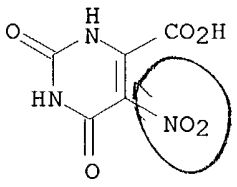


Same as #25

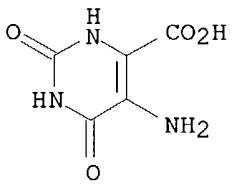
IT **7164-43-4D**, transition metal complexes
RL: PRP (Properties)
(spectra of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 74 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:463173 CAPLUS
DN 99:63173
TI Coordination sites of 5-nitro-6-carboxyuracil: UV study and x-ray structure determination of diammine(5-nitroorotato)copper(II) hydrate and hexaamminebis(5-nitroorotato)tricopper(II) pentahydrate
AU Arrizabalaga, Philippe; Castan, Paule; Dahan, Francoise
CS Lab. Chim. Coordination, Univ. Paul Sabatier, Toulouse, 31400, Fr.
SO Inorganic Chemistry (1983), 22(16), 2245-52
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
AB A systematic study of UV spectra of 5-nitroorotic acid (H3L), for various pH values, shows that in the presence of metal ions (Cu(II)) the ligand is fully deprotonated. Cu(NH3)2(HL).H2O (I) and Cu3(NH3)6L2.5H2O (II) were prepared and investigated. Both complexes crystallize in the monoclinic system. Crystal data for I: space group P21/c, a 10.417(2), b 7.212(1), c 14.378(3)Å, β 94.30(2)°, V = 1077.2 Å3, Z = 4, 1806 reflections, R = 0.036. Crystal data for II: space group C2/c, a 18.823(3), b 7.329(1), c 20.081(6) Å, β 105.33(2)°, V = 2671.5 A3, Z = 4, 2216 reflections, R = 0.054. These studies give the first evidence that an orotic acid derivative can coordinate the Cu2+ ion simultaneously by the 2 N sites of the completely deprotonated ligand.
IT **17687-24-0**
RL: PRP (Properties)
(UV spectrum of, pH effects on)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



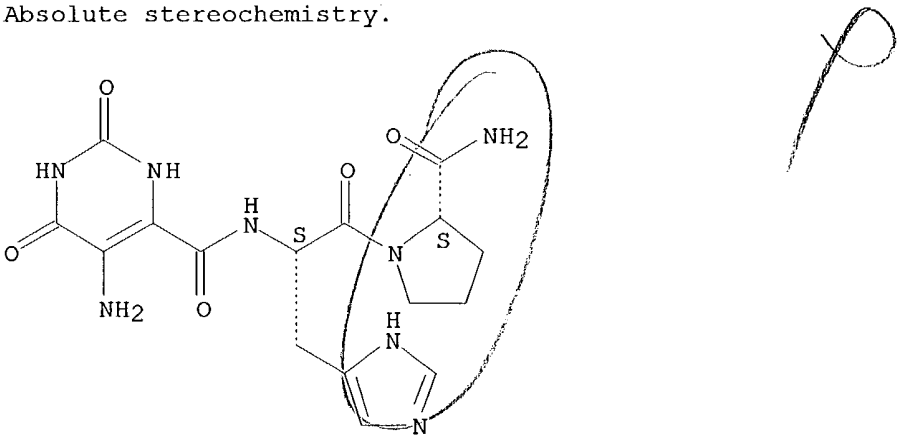
L6 ANSWER 76 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:156890 CAPLUS
DN 98:156890
TI Enzymes of the de novo pyrimidine biosynthetic pathway in Toxoplasma gondii
AU Asai, Takashi; O'Sullivan, William J.; Kobayashi, Masashi; Gero, Annette M.; Yokogawa, Muneo; Tatibana, Masamiti
CS Sch. Med., Chiba Univ., Chiba, 280, Japan
SO Molecular and Biochemical Parasitology (1983), 7(2), 89-100
CODEN: MBIPDP; ISSN: 0166-6851
DT Journal
LA English
AB All 6 enzymes of the de novo biosynthetic pathway leading to the biosynthesis of UMP were characterized in T. gondii. The first 3 enzymes of the pathway, carbamyl phosphate synthetase-II (CPS-II), aspartate transcarbamylase (ATCase) and dihydroorotase (DHOase) were consistently separated by sucrose gradient centrifugation. Their mol. wts. were .apprx.540,000, 140,000 and 70,000, resp. The last 2 enzymes, orotate phosphoribosyltransferase (OPRTase) and orotidylate decarboxylase (ODCase), cosedimented at the same position, corresponding to a mol. weight of .apprx.70,000. The 4th enzyme, dihydroorotate dehydrogenase (DHO-DHase), was associated with the particulate fraction. Apparent Km values for the resp. enzymes were: CPS-II, MgATP2- (19.7 mM), L-glutamine (12.0 μM), NH3 (15.5 mM); ATCase, carbamyl phosphate (26.2 μM), L-aspartate (17.6 mM); DHOase (reverse direction) dihydroorotate (1.6 μM); ODCase, orotidine 5'-monophosphate (0.41 μM). MgUTP2- was an inhibitor of CPS-II, with an apparent Ki of 0.41 mM. However, 5-phospho-α-D-ribosyl 1-diphosphate, DMSO, and glycerol had no effect on the Km for MgATP2-. The effect of some inhibitors, including pyrimidine and purine nucleotides and analogs and respiratory chain inhibitors, was also determined for the enzymes of the pathway.
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

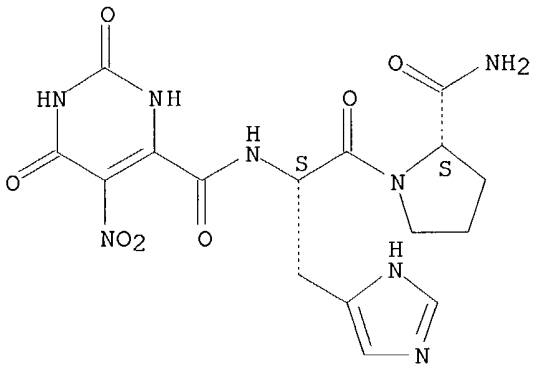
L6 ANSWER 77 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:65794 CAPLUS
DN 98:65794
TI Biological effects of degradation-stabilized TRH analogs
AU Flohe, L.; Bauer, K.; Friderichs, E.; Gunzler, W. A.; Hennies, H. H.; Herrling, S.; Lagler, F.; Otting, F.; Schwertner, E.
CS Cent. Res., Grunenthal G.m.b.H., Aachen, D-5100, Fed. Rep. Ger.
SO Thyrotropin-Releasing Horm. (1983), 327-40. Editor(s): Griffiths, E. C.; Bennett, G. W. Publisher: Raven, New York, N. Y.
CODEN: 48ZRAE
DT Conference
LA English
AB TRH analogs in which the pyroglutamyl residue was displaced by 5- or 6-membered ring systems were resistant to TRH-degrading enzymes, frequently showed central nervous system effects qual. similar to those of TRH [24305-27-9], and (with 1 exception) were endocrinol. less active. CG 3703 (I) [90243-66-6] was much more potent than TRH with regard to both pharmacol. and endocrinol. activities. Structure-activity relations for the analogs are discussed.
IT **84458-57-1 84458-58-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(biol. activity of, mol. structure in relation to)
RN 84458-57-1 CAPLUS
CN L-Prolinamide, N-[(5-amino-1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinyl)carbonyl]-L-histidyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

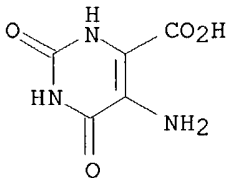


RN 84458-58-2 CAPLUS
CN L-Prolinamide, N-[(1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-4-pyrimidinyl)carbonyl]-L-histidyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

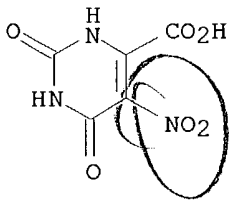


L6 ANSWER 78 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:616435 CAPLUS
DN 97:216435
TI Study of the slow protonation of the complexes between divalent nickel ion and dianion of orotic acid or its derivatives
AU Lalart, Denis; Dodin, Guy; Dubois, Jacques-Emile
CS Inst. Topol. Dyn. Syst., Univ. Paris VII, Paris, 75005, Fr.
SO Journal de Chimie Physique et de Physico-Chimie Biologique (1982), 79(5), 449-53
CODEN: JCPBAN; ISSN: 0021-7689
DT Journal
LA French
AB Addition of Ni2+ ions to alkaline or neutral solns. of orotic acid (I) or its 5-substituted derivs. gives 1:1 complexes with the dianion. The rate constant of this reaction is independent of the ligand. The dissociation of these complexes in acidic media occurs via a mechanism which involves slow protonation of the complexes instead of the expected faster diffusion-limited rate. The relative weight of the 2 reaction paths depends on the substituent at position 5 of I.
IT **7164-43-4 17687-24-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with nickel ions)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

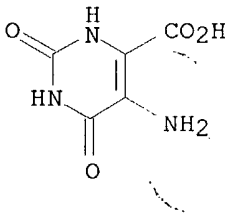


Saw on #25

RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 80 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:2855 CAPLUS
DN 96:2855
TI Comparative studies on dihydroorotate dehydrogenase from P. berghei and the mouse reticulocyte
AU Gero, Annette M.; Finney, Kenneth G.; Bennett, Julie C.; O'Sullivan, William J.
CS Sch. Biochem., Univ. New South Wales, Kensington, 2033, Australia
SO Australian Journal of Experimental Biology and Medical Science (1981), 59(4), 477-90
CODEN: AJEBAK; ISSN: 0004-945X
DT Journal
LA English
AB Kinetic parameters of dihydroorotate dehydrogenase (DHO-DHase) from the rodent malarial parasite, Plasmodium berghei, were determined This enzyme, the 4th in de novo pyrimidine biosynthesis, is particulate and is absent from the mature mammalian red cell. The Km of the substrate, dihydroorotate, was determined to be 23 μM and the Ki values for a number of substrate analogs were determined The most potent inhibitor was dihydroazaorotate (Ki, 3 μM). The product orotate was also a good inhibitor (Ki, 5 μM) as were methylorotate (Ki, 10 μM), 5-azaorotate (Ki, 20 μM) and other pyrimidine analogs. The activity of the enzyme was also affected by a number of respiratory chain inhibitors. Since the P. berghei infection is accompanied by reticulocytosis, a comparative study of DHO-DHase in mouse reticulocytes was also carried out. The general properties of the enzyme from these sources were similar to those of the parasite enzyme. However, significant differences in the response of the 2 enzymes to various inhibitors were observed and could provide a rational basis for the development of chemotherapeutic agents active against the parasite.
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



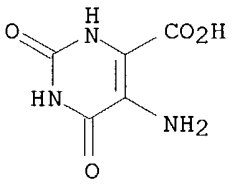
Same as #25

L6 ANSWER 81 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:407314 CAPLUS
DN 95:7314
TI 2,6-Bis(diethanolamino)-4,8-dipiperidinopyrimido[5,4-d]pyrimidine
IN Margineanu, Dan Axente
PA Fed. Rep. Ger.
SO Ger. Offen., 4 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 2927539	A1	19810108	DE 1979-2927539	19790707
PRAI DE 1979-2927539		19790707		

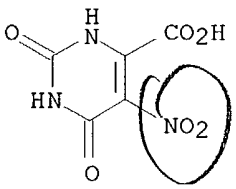
AB The title compound [I; R = N(CH2CH2OH)2, R1 = piperidino] was prepared by condensing urea with MeCOCH2CO2Me, nitrating 6-methyluracil, oxidizing 6-methyl-5-nitrouracil, reducing the NO2 group in nitroorotic acid, condensing aminoorotic acid with urea, chlorinating I (R = R1 = OH), and aminating I (R = R1 = Cl).

IT **7164-43-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with urea)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

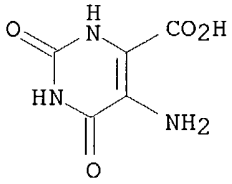


Same as #25

IT **17687-24-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

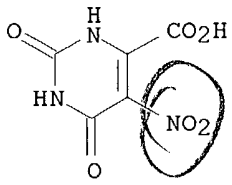


L6 ANSWER 82 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:421532 CAPLUS
DN 93:21532
TI The effects of pH and inhibitors upon the catalytic activity of the dihydroorotase of multienzymic protein pyrl-3 from mouse Ehrlich ascites carcinoma
AU Christopherson, Richard I.; Jones, Mary Ellen
CS Sch. Med., Univ. North Carolina, Chapel Hill, NC, 27514, USA
SO Journal of Biological Chemistry (1980), 255(8), 3358-70
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
AB Factors affecting the catalytic activity of dihydroorotase (EC 3.5.2.3) (I), purified as part of a multienzymic protein which contains carbamyl phosphate synthetase, aspartate transcarbamylase, and I (ME pyrl-3) and which initiates de novo pyrimidine biosynthesis in mouse Ehrlich ascites carcinoma, were studied. The apparent Km for N-carbamyl-L-aspartate (II) increased by 2 orders of magnitude as the pH increased from 7.0 to 8.3, consistent with equilibration of I (E) between 4 states of protonation (E .dblarw. EH .dblarw. EH2 .dblarw. EHh3), where EH3 is the only catalytically active form of I for the biosynthetic reaction, having a Km for II of 30 μM. The apparent Km for L-5,6-dihydroorotate (III) showed a converse dependence upon pH, remaining relatively constant at alkaline pH and increasing progressively as the pH was decreased below 7.0. These data were consistent with the above model if E and EH are catalytically active for the degradative reaction, both having Km values of 4.4 μM for III. The D isomers of carbamylaspartate and dihydroorotate were also substrates for I. At pH 7.33, the apparent Km values for II and N-carbamyl-D-aspartate were 247 and 204 μM, resp., but the Vmax for N-carbamyl-D-aspartate was only 1.7% of that obtained with II. Orotate and a series of 5-substituted derivs. were competitive inhibitors of I. At pH 7.27, the apparent Ki for orotate using II as substrate was 170 μM and with III as substrate, the apparent Ki was 9.6 μM, suggesting that the enzyme exists in different forms in the presence of each substrate. I was inhibited in a time-dependent manner by 50 mM L-cysteine and the presence of II or III protected against this ultimately complete inactivation. 2-Mercaptoacetate, 2-mercaptoethylamine, 3-mercaptopropionate, and L-2,3-diaminopropionate had a similar although less potent inhibitory effect. To account for the data obtained, a model for the equilibrium existing between various protonated forms of I was proposed, which was with the pH dependencies of the apparent Km values observed and the Vmax values observed previously. In addition, a catalytic mechanism was presented for the interconversion of II and III.
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotase inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

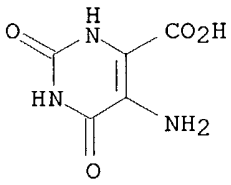


Same as #25

L6 ANSWER 83 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1979:523248 CAPLUS
DN 91:123248
TI Acid-base properties of uracil and its derivatives in a dimethylsulfoxide medium
AU Mikstais, U.; Smolova, N. T.; Veveris, A.; Jurgevica, I.
CS Vses. Nauchno-Issled. Inst. Prikl. Biokhim., Olaine, USSR
SO Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1979), (3), 324-7
CODEN: LZAKAM; ISSN: 0002-3248
DT Journal
LA Russian
AB The pKa values of uracil and its 5-Br, 5-NO2, 2-thio, and 5,6-dihydro derivs. were 12.8, 10.7, 6.8, 10.6, and 16.1, resp. Those of the corresponding uracil-6-carboxylic acids varied from 3.5 to 8.6 for the CO2H group and from 10.4 to 16.3 for the NH group.
IT **17687-24-0**
RL: PRP (Properties)
(pKa of, in Me sulfoxide)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

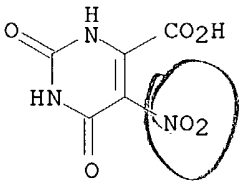


L6 ANSWER 84 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:592878 CAPLUS
DN 89:192878
TI A simple radioassay for dihydroorotate dehydrogenase
AU Smithers, G. W.; Gero, Annette M.; O'Sullivan, W. J.
CS Sch. Biochem., Univ. New South Wales, Kensington, Australia
SO Analytical Biochemistry (1978), 88(1), 93-103
CODEN: ANBCA2; ISSN: 0003-2697
DT Journal
LA English
AB A simple radioassay for dihydroorotate dehydrogenase (I) was developed. L-Dihydroorotate-carboxy-14C was prepared from orotic acid-carboxy-14C using I derived from Zymobacterium oroticum and was purified by elution from DEAE-Sephadex A-25 with 0.2M ammonium formate, pH 7. I activity in human spleen mitochondria was determined by the release of 14CO2 from the carboxy-14C-labeled L-dihydroorotate, the reaction being coupled with added orotate phosphoribosyltransferase and orotidylate decarboxylase. An apparent Km value of .apprx.5 μM for L-dihydroorotate was established using the radioassay.
IT **7164-43-4**
RL: BIOL (Biological study)
(dihydroorotate dehydrogenase inhibition by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as #25

L6 ANSWER 85 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:535819 CAPLUS
DN 89:135819
TI Preparation of pure 5-nitrouracil-6T and 5-cyanouracil-6T
AU Heise, K. H.; Noll, S.
CS Zentralinst. Kernforsch. Rossendorf, DAW, Rossendorf, Ger. Dem. Rep.
SO Zentralinst. Kernforsch., Rossendorf Dresden, [Ber.] (1977), ZfK-340, Jahresbericht, 83-4
CODEN: ZKRDBY
DT Report
LA German
AB 5-Nitrouracil-6-3H (I) [67695-03-8] and 5-cyanouracil-6-3H (II) [67695-04-9] were prepared to investigate the kinetics of 3H-labeling of 5-position derivs. of uracil, useful in biol. and pharmacol. studies. I was prepared by a modified method of Filip, Vysata and Farkas. 5-Nitroorotic acid [**17687-24-0**] was labeled with tritiated H2O and then decarboxylated in anhydrous dioxane at 100° to give a 69% yield of I with 63.5% labeling yield. II was prepared from 5-cyanouracil by acid-catalyzed H-3H exchange in 50% aqueous trifluoroacetic acid-3H for 300 h in 50.8% yield. A 1000 h reaction time gave only a 27.1% yield, but a 76% labeling yield. II was prepared more conveniently from 5-aminouracil-6-3H [67695-05-0] by the Sandmeyer reaction in the presence of CuCN.
IT **17687-24-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(tritium-labeling and decarboxylation of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

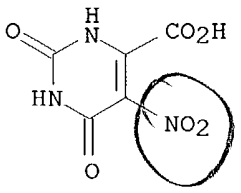


L6 ANSWER 86 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:89711 CAPLUS
DN 88:89711
TI 5-Nitrouracil-4-carboxylic acid
IN Goldner, Herbert; Krahnefeld, Helmut; Sauer, Wolfgang; Carstens, Ernst; Wolf, Josef; Scharnagel, Werner; Stutzriemer, Siegfried; Trobisch, Siegfried
PA Ger. Dem. Rep.
SO Ger. (East), 7 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 126811	Z	19770817	DD 1976-194113	19760729
PRAI DD 1976-194113		19760729		

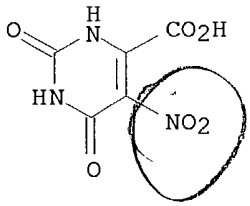
AB The title compound was prepared by dissolving 1 mol 4-methyluracil (I) in H2SO4, nitrating I with 1.34 mol HNO3 at room temperature, whereby the temperature slowly rises to 40°, and, without isolation, oxidizing the product 4-methyl-5-nitrouracil with 3.36 mol HNO3 during 45-60 min at 40-50°. The temperature was allowed to rise to 55-60°, then kept at 60-5°, finally 90-5° to give the title compound, characterized as the K salt.

IT **65717-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65717-13-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, monopotassium salt (9CI) (CA INDEX NAME)



● K

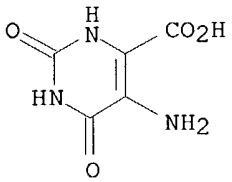
L6 ANSWER 87 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:44544 CAPLUS
DN 88:44544
TI Potentiometric determination of orotic acid in mixtures with its derivatives
AU Veveris, A.; Mikstais, U.; Jurgevica, I.
CS Vses. Nauchno-Issled. Inst. Prikl. Biokhim., Olaine, USSR
SO Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1977), (4), 498
CODEN: LZAKAM; ISSN: 0002-3248
DT Journal
LA Russian
AB Binary mixts. of orotic acid, its 6-carboxybutyl, 5,6-dihydro, 2-thio, and 5-nitro derivs. were analyzed by potentiometric titration in Me2CO with 0.1N Et4NOH in iso-PrOH. The relative error was ≤1.2%.
IT **17687-24-0**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in mixts. with orotic acid by nonaq. potentiometric titration)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 88 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:37832 CAPLUS
DN 88:37832
TI 5-Aminoorotic acid
IN Giacobini, Valeriano
PA Lonza A.-G., Switz.
SO Patentschrift (Switz.), 2 pp.
CODEN: SWXXAS
DT Patent
LA German
FAN.CNT 2

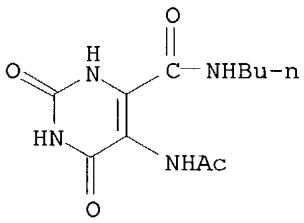
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CH 592636	A	19771031	CH 1975-423	19750113
	DE 2600542	A1	19760715	DE 1976-2600542	19760108
	DE 2600542	C2	19860109		
PRAI	CH 1975-423		19750113		

AB 5-Aminoorotic acid was obtained quant. by reducing K 5-nitroorotate with Pd-C.
IT **7164-43-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



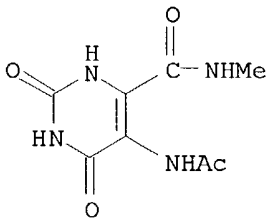
Same as # 25

L6 ANSWER 89 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:484935 CAPLUS
DN 87:84935
TI Synthesis and properties of some new derivatives of pyrimido[5,4-d]pyrimidine
AU Britikova, N. E.; Elina, A. S.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1977), (4), 517-20
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
OS CASREACT 87:84935
AB Pyrimidopyrimidinetriones I (R = Bu, Me, HOCH2CH2) were prepared in 47-61% yields by thermal cyclization. I (R = Bu) was chlorinated by POCl3 to give 71% II (R1 = R2 = Cl), which was aminated to give 60-94% II (R1 = piperidino, Et2N, NH2, PhCH2NH, Me2CHNH, 1-cyclohexen-1-ylethylamino, R2 = Cl). Addnl. obtained from II (R1 = R2 = Cl) were 57-96% II [R1 = R2 = BuNH, MeO, SH, SMe; R1 = NH2, R2 = OMe, SH, SMe; R1 = piperidino, R2 = N(CH2CH2OH)2].
IT **63656-48-4P 63656-49-5P 63656-50-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal cyclization of)
RN 63656-48-4 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-N-butyl-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

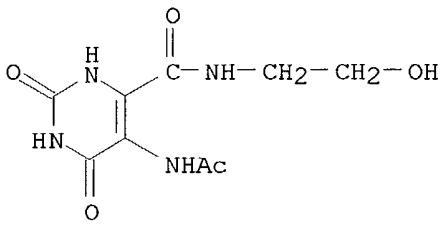


Intermediates

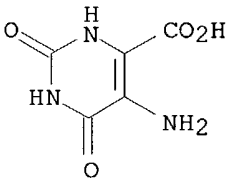
RN 63656-49-5 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-1,2,3,6-tetrahydro-N-methyl-2,6-dioxo- (9CI) (CA INDEX NAME)



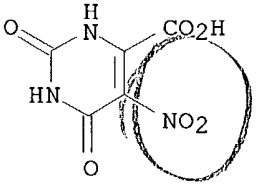
RN 63656-50-8 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-1,2,3,6-tetrahydro-N-(2-hydroxyethyl)-2,6-dioxo- (9CI) (CA INDEX NAME)



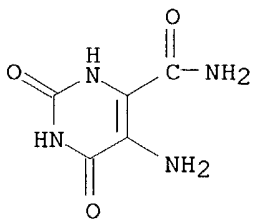
L6 ANSWER 90 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:152007 CAPLUS
DN 86:152007
TI Inhibition of uricase by substituted pyrimidines
AU Sedor, Frank A.; Sander, Eugene G.
CS Sch. Med., West Virginia Univ., Morgantown, WV, USA
SO Biochemical and Biophysical Research Communications (1977), 75(2), 406-13
CODEN: BBRCA9; ISSN: 0006-291X
DT Journal
LA English
AB Twenty-eight pyrimidine derivs. were tested for their ability to inhibit uricase (I) at pH 8.5. Half of the compds. competitively inhibited I with Ki values of 4.4 + 10-4 - 4.2 + 10-6 M. Qual., there is a relation between the degree of electron-withdrawing ability of substituents at C-5 of the pyrimidine ring system and the magnitude of inhibitor interaction with I, apparently due to the binding of pyrimidine anions rather than the binding of the protonated species.
IT **7164-43-4 17687-24-0**
RL: BIOL (Biological study)
(uricase inhibition by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 91 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:592654 CAPLUS
DN 85:192654
TI An improved synthesis of pyrimido[5,4-d]pyrimidine derivatives substituted by mercapto groups
AU Inukai, Noriyoshi; Katuno, Keishi; Ishii, Yasuo; Ishii, Yoshio; Uda, Mituru; Murakami, Masuo
CS Cent. Res. Lab., Yamanouchi Pharm. Co., Ltd., Tokyo, Japan
SO Chemical & Pharmaceutical Bulletin (1976), 24(7), 1506-9
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
OS CASREACT 85:192654
AB 5-Amino-6-hydroxy-2-(methylthio)pyrimidine-4-carboxamide (I) was prepared from Me 6-hydroxy-2-(methylthio)pyrimidine-4-carboxylate by bromination, followed by amino amidation. I was also prepared by a similar treatment of 6-hydroxy-2-(methylthio)pyrimidine-4-carboxamide, which was synthesized by half-amidation of Na salt of Et Me oxalacetate, followed by treatment with S-methylisothiourea sulfate. 4,8-Dihydroxy-2-mercapto-6-(methylthio)pyrimido[5,4-d]pyrimidine (II) was prepared quant. by refluxing I with Na or K ethylxanthate or with diethylammonium N,N-diethyldithiocarbamate in suitable solvents, such as pyridine and water. II was converted to 4,8-dihydroxy-2,6-dimercaptopyrimido[5,4-d]pyrimidine by treating the Na salt of II in ethylene glycol at about 125° with H2S.
IT **60988-09-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with ethyl xanthate, pyrimidopyrimidines from)
RN 60988-09-2 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



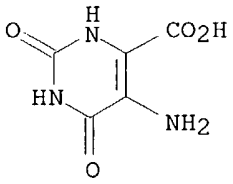
Intermediate

L6 ANSWER 92 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:577481 CAPLUS
DN 85:177481
TI 5-Aminoorotic acid
IN Giacobini, Valeriano
PA Lonza Ltd., Switz.
SO Ger. Offen., 5 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

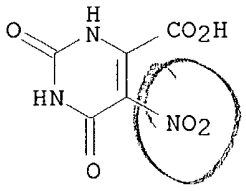
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2600542	A1	19760715	DE 1976-2600542	19760108
	DE 2600542	C2	19860109		
	CH 592636	A	19771031	CH 1975-423	19750113
PRAI	CH 1975-423		19750113		

AB Reduction of 5-nitroorotic acid K salt in aqueous KOH over Pd/C (5% Pd) at 30-40° and 7-9 atm H2 pressure gives quant. 5-aminoorotic acid, an intermediate in manufacture of dipyridamole.

IT **7164-43-4P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

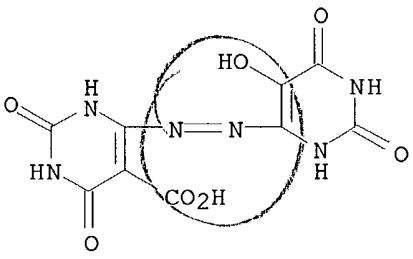


IT **60779-49-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 60779-49-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, potassium salt (9CI) (CA INDEX NAME)

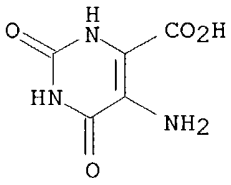


●x K

L6 ANSWER 93 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:523008 CAPLUS
DN 85:123008
TI Electrochemical oxidation of 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-d]pyrimidine-4,6-dione (oxipurinol) at the pyrolytic graphite electrode
AU Dryhurst, Glenn
CS Dep. Chem., Univ. Oklahoma, Norman, OK, USA
SO Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1976), 70(2), 171-97
CODEN: JEIEBC; ISSN: 0022-0728
DT Journal
LA English
AB The electrochem. oxidation of 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-d]pyrimidine-4,6-dione (I) at the pyrolytic graphite electrode exhibits up to three voltammetric oxidation peaks between pH 1-12. The first pH-dependent peak is an initial, irreversible 2e--2H+ reaction to give 5,6-dihydro-4H-pyrazolo[3,4-d]pyrimidine-4,6-dione II, which further reacts by two routes. The major route (90%) involves a Michael addition of water followed by further electrochem. oxidation and hydrolysis to give 5,6-dihydro-5,6-dihydroxy-5-carboxy-6-diazenouracil (III). The minor route involves further electrochem. oxidation of II in a 2e--2H+ reaction to give 4,5,6,7-tetrahydro-3H-pyrazolo[3,4-d]-pyrimidine-3,4,6-trione (IV).
IT **60450-60-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60450-60-4 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-2,4-dioxo-6-[(1,2,3,6-tetrahydro-5-hydroxy-2,6-dioxo-4-pyrimidinyl)azo]- (9CI) (CA INDEX NAME)

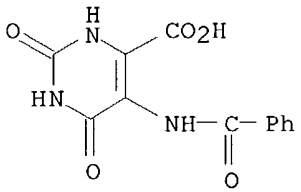


L6 ANSWER 94 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:432948 CAPLUS
DN 85:32948
TI Synthesis of 2,4-disubstituted 5-aminopyrimidine-6-carboxylic acids derivatives. Part I.
AU Machon, Zdzislaw; Jasztold-Howorko, Ryszard
CS Inst. Chem. Technol. Drugs, Med. Acad., Wroclaw, Pol.
SO Polish Journal of Pharmacology and Pharmacy (1976), 28(1), 61-7
CODEN: PJPPAA; ISSN: 0301-0244
DT Journal
LA English
AB Pyrimidinecarboxylic acid derivs. I (R = R1 = NH2, NEt2, NHPh, cyclohexylamino, NHC6H4Cl-4, NHC6H4OEt-4; R = NEt2, NHPh, cyclohexylamino, NHC6H4OEt-4, R1 = OEt; R = NHC6H4OEt-4, R1 = OH) were prepared by N-benzoylating 5-aminoorotic acid, treating the N-benzoyl derivative with POCl3, treating the lactam II with NaOH, EtOH, or amines to give I (R = Cl, R1 = OH, OEt, R = R1 = amino resp.) and treating I (R = Cl) with amines. None of the products showed any antiinflammatory or virucidal acitivity.
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzoylation of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



Same as before -

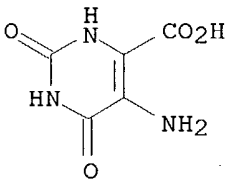
IT **59662-86-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 59662-86-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



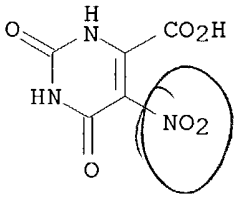
L6 ANSWER 95 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:421447 CAPLUS
DN 85:21447
TI 2,4,6,8-Tetrahydroxypyrimido[5,4-d]pyrimidine
IN Knoll, Gottfried; Goldner, Herbert; Krahnefeld, Helmut
PA Ger. Dem. Rep.
SO Ger. (East), 7 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DD 117457	Z	19760112	DD 1975-184154	19750213
PRAI	DD 1975-184154		19750213		

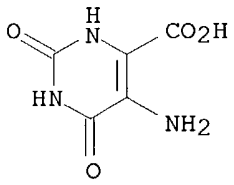
AB The title compound was obtained in 75% yield by condensing 5-aminouracil-4-carboxylic acid containing 44% H2O with urea.
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with urea)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



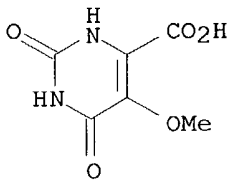
L6 ANSWER 96 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:73252 CAPLUS
DN 84:73252
TI ESR study of the anion radicals of 5-nitropyrimidines: conversion to iminoxy radicals
AU Sevilla, M. D.; Clark, C.; Failor, R.
CS Dep. Chem., Oakland Univ., Rochester, MI, USA
SO Radiation Research (1976), 65(1), 29-40
CODEN: RAREAE; ISSN: 0033-7587
DT Journal
LA English
AB The anion radicals of 5-nitropyrimidines were examined by ESR spectroscopy. The anions are formed by electrolysis in DMF and by electron attachment in aqueous glasses, 12 M LiCl-D2O and 8 M NaOD. The electrolysis of 5-nitrouracil and 5-nitro-6-methyluracil results in relatively stable anion radicals. The results for 5-nitrouracil give evidence for two or perhaps three anions which differ only by the degree of ring N protonation. The results for 5-nitro-6-methyluracil suggest that the nitro group of the anion is twisted so that it is coupled only weakly to the ring π-electron system. The anions of 5-nitrouracil, 5-nitroorotic acid, 5-nitrobarbituric acid, and 5-nitro-6-methyluracil were produced in the alkaline and neutral aqueous glasses. The anisotropic spectra were analyzed with the aid of computer simulations which assume axial symmetry. A concentration dependence in the splittings is noted and discussed. Uv photolysis of the anions of 5-nitro-6-methyluracil and 5-nitrobarbituric acid results in iminoxy radicals. Mechanisms of formation of the iminoxy radicals are discussed and the results are compared to those found in single crystals and aqueous solution
IT **58431-14-4**
RL: PRP (Properties)
(ESR of)
RN 58431-14-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, radical ion(1-) (9CI) (CA INDEX NAME)



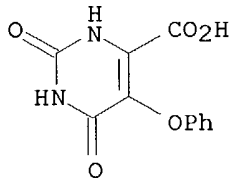
L6 ANSWER 97 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:30998 CAPLUS
DN 84:30998
TI Synthesis of new physiologically active derivatives of pyrimido[5,4-d]pyrimidine
AU Golomolzin, B. V.; Anoshina, G. M.
CS Ural. Politekh. Inst. im. Kirova, Sverdlovsk, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (1975), 9(10), 17-19
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
AB Pyrimidopyrimidines I (R = H, o-MeO, p-Cl) were obtained in 33-52% yields by condensation of 5-aminoorotic acid with RC6H4NCS or RC6H4NHCSNH2 2 hr in boiling DMF. Treatment of I (R = H) with N2H4.H2O gave 35% II.H2O. I were useful as neoplasm inhibitors.
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenyl isothiocyanates or phenylthioureas)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



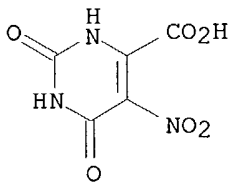
L6 ANSWER 98 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:57638 CAPLUS
DN 82:57638
TI Unsaturated hydantoin derivatives. XI. Synthesis and rearrangement of some ethyl esters of α-substituted hydantoin-Δ5,α-acetic acids
AU Ivin, B. A.; Rutkovskii, G. V.; Rusavskaya, T. N.; Smorygo, N. A.; Sochilin, E. G.
CS Leningr. Tekh. Inst. im. Lensoveta, Leningrad, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1974), (11), 1527-35
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
AB Hydantoins (I; R = H, Me, Ph; R1 = H, Me, MeO, Ph, PhO, F, Cl, NO2, OH) were prepared by condensation of H2NCONHR with EtO2CC(OH):CR1CO2Et at 100° in AcOH. Heating I 1 hr at 100° with KOH gave 55-98% yields of orotic acids (II; R2 = H, Me; Ph; R3 = H, Me, Ph, OPh, OMe, F, Cl, NO2).
IT **6944-35-0P 14383-34-7P 17687-24-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 6944-35-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-methoxy-2,6-dioxo- (9CI) (CA INDEX NAME)



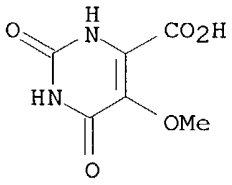
RN 14383-34-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-phenoxy- (9CI) (CA INDEX NAME)



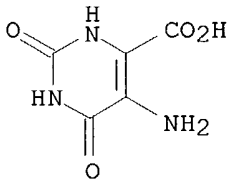
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 99 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:11023 CAPLUS
DN 82:11023
TI In vitro antimalarial activity of nucleic acid precursor analogs in the simian malaria Plasmodium knowlesi
AU McCormick, Gerald J.; Canfield, Craig J.; Willet, Gloria P.
CS Div. Med., Walter Reed Army Inst. Res., Washington, DC, USA
SO Antimicrobial Agents and Chemotherapy (1974), 6(1), 16-21
CODEN: AMACCQ; ISSN: 0066-4804
DT Journal
LA English
AB Incorporation of adenosine or orotic acid into P. knowlesi nucleic acids in vitro was effectively inhibited by many nucleic acid precursor analogs, including 3' analogs of purine nucleosides, many of the 6-position analogs of purine bases and nucleosides, and 5-position analogs of orotic acid. Only a few compds. inhibited methionine incorporation into protein, and in each instance adenosine or orotic acid incorporation also was inhibited. Some compds. inhibited adenosine or orotic acid incorporation into both RNA and DNA whereas others inhibited incorporation into one nucleic acid only. The qual. and quant. differences suggest that this exptl. system may be appropriate for investigation or metabolic pathways of the malaria parasite, as well as for demonstration of antimalarial activity of candidate antimalarial drugs.
IT **6944-35-0 7164-43-4 17687-24-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antimalarial activity of)
RN 6944-35-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-methoxy-2,6-dioxo- (9CI) (CA INDEX NAME)

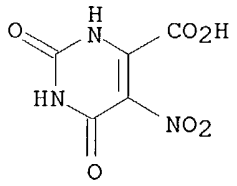


RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

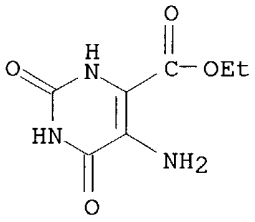


RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI)

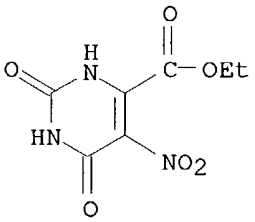
(CA INDEX NAME)



L6 ANSWER 100 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:133381 CAPLUS
DN 80:133381
TI Syntheses of N-heterocyclic compounds. XVIII. Syntheses of disubstituted amino-2-phenylpyrimido-pyrimidine derivatives
AU Yurugi, Shojiro; Miyake, Akio; Tada, Norio
CS Takeda Chem. Ind., Ltd., Osaka, Japan
SO Takeda Kenkyushoho (1973), 32(3), 251-8
CODEN: TAKHAA; ISSN: 0371-5167
DT Journal
LA Japanese
AB Hofmann rearrangement of 2-phenylpyrimidine-4,5-dicarboxamide (I) gave a mixture of 5,7-dihydroxy-2-phenylpyrimido[4,5-d]pyrimidine (II) and 6,8-di-hydroxy-2-phenylpyrimido[5,4-d]pyrimidine (III). II was also prepared by the reaction of 4-amino-5-carbamoyl-2-phenylpyrimidine (IV) with urea. Among the disubstituted amino compds. derived from II and III, 5,7-dimorpholino-2-phenylpyrimido-[4,5-d]pyrimidine (V) showed diuretic activity.
IT **40598-01-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40598-01-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)

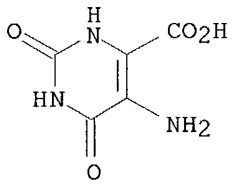


IT **52047-16-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 52047-16-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure of, with benzamidine)
RN 7164-43-4 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



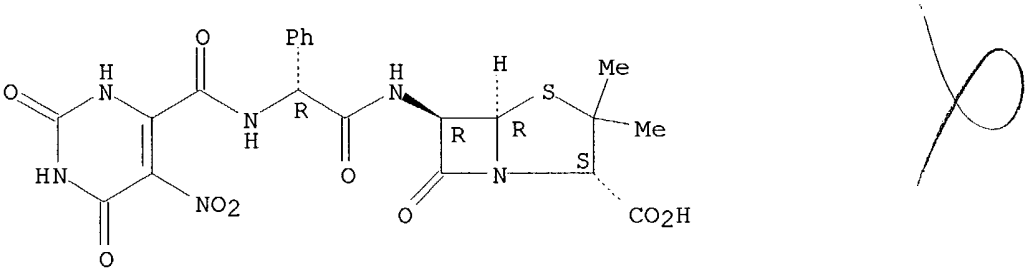
L6 ANSWER 101 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:108504 CAPLUS
DN 80:108504
TI α-Acylaminobenzylpenicillins
IN Kawahara, Norio; Murakami, Masuo; Isaka, Ichiro; Horiguchi, Hiroshi; Murakami, Yukiyasu; Kashiwagi, Teruya
PA Yamanouchi Pharmaceutical Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 49000292	A2	19740105	JP 1972-39914	19720420
PRAI JP 1972-39914		19720420		

AB The title compds. (I) [R1,2 = H, NH2, acylamino, alkylamino, OH, alkoxy, SH, or alkylthio; R3 = NO2, halogen, CN, HCO, NH2, acylamino, alkylamino, OH, alkoxy, SH, alkylthio, or alkyl), useful as antibacterials, were prepared by treating α-aminobenzylpenicillin (II) with pyrimidines (III) or reactive derivs. thereof. E.g., 4 g II.3H2O in CH2Cl2 was treated with 35 ml NEt3 in the presence of MgSO4, the resulting II.NEt3 solution treated with 2.2 g III (R1 = R2 = OH, R3 = NO2) (acid chloride) with cooling, and treated with K 2-ethylhexanoate to give 56.7% K salt of D-I (R1-R3 the same as before). Similarly prepared was the Na salt of D-I (R1 = R2 = OH, R3 = Br).

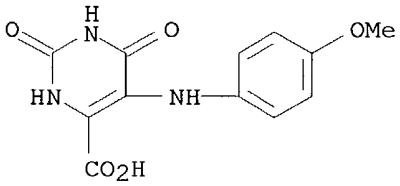
IT **52265-98-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52265-98-2 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[(1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-4-pyrimidinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monopotassium salt, [2S-[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



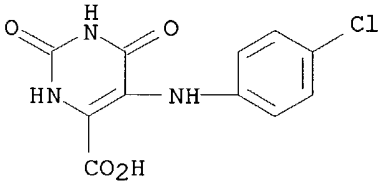
● K

L6 ANSWER 102 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:95875 CAPLUS
DN 80:95875
TI Pyrimido[5,4-b]quinoline derivatives
AU Britikova, N. E.; Belova, L. A.; Magidson, O. Yu; Elina, A. S.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1974), (1), 131-3
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
AB Pyrimidoquinoline I (R1 = R2 = H, R3 = MeO) was obtained in 67% yield by heating the appropriate pyrimidinedione (II) with POCl3 1 hr at 80°. Pyrimidoquinolines (III; R1 = H, Me, R2 = H, Me, R3 = OMe, H, Cl, R4 = Cl) were obtained in 34-60% yields by boiling II with POCl3 3 hr at 80-90°. Addnl. obtained were III (R1 = R2 = R3 = H, R4 = morpholino, PhCH2NH; R1 = R2 = H, R3 = Cl, R4 = morpholino).
IT **6964-60-9 40598-18-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosphorus oxychloride)
RN 6964-60-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(4-methoxyphenyl)amino]-2,6-dioxo- (9CI) (CA INDEX NAME)

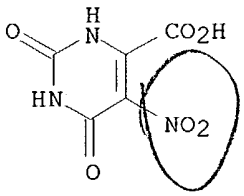


Sy Sept

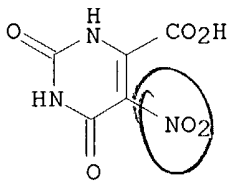
RN 40598-18-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorophenyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



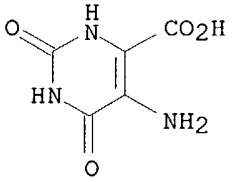
L6 ANSWER 103 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:415195 CAPLUS
DN 79:15195
TI Electron spin resonance and pulse radiolysis studies of irradiated aqueous solutions of 5-nitrouracils. Oxidative denitration by hydroxyl radicals
AU Neta, P.; Greenstock, C. L.
CS Mellon Inst. Sci., Carnegie-Mellon Univ., Pittsburgh, PA, USA
SO Radiation Research (1973), 54(1), 35-48
CODEN: RAREAE; ISSN: 0033-7587
DT Journal
LA English
AB Radicals produced in irradiated aqueous solns. of 5-nitrouracil, 5-nitroorotic acid, and 5-nitrobarbituric acid have been studied by the in situ radiolysis steady state ESR method and the kinetics of their formation and disappearance were followed by pulse radiolysis. The reactions of hydroxyl radicals with 5-nitrouracil and its derivs. are nearly diffusion controlled and involve addition of OH to the 5,6 double bond. Addition of OH to the C bearing the nitro group leads to oxidative denitration by subsequent rapid elimination of HNO2. This reaction is analogous to dehalogenation following OH addition to 5-halouracils, and the radicals produced from both the nitro and the halo compds. are identical. Addition of OH to position 6 is also important, but the radicals formed were not observed by ESR. The distribution of OH addition between position 5 and 6 was determined by the pulse radiolysis expts. and found to involve 25 and 30% addition to the 5 position of 5-nitrouracil and 5-nitrobarbituric acid, resp., i.e., in these two cases the efficiency of oxidative denitration is 25-30%. The transient optical absorption spectra recorded immediately after the reaction of OH with 5-nitrouracil, 5-bromouracil, and isobarbituric acid are very similar and are attributed to the same radical. The rate of reaction of OH has been monitored both by the buildup of the transient absorption and by the destruction of the parent compound absorption, and the two measurements give rate consts. of 7 ± 2 + 109M-1 sec-1 for the four nitrouracil derivs. examined These findings indicate that denitration, like dehalogenation, occurs rapidly following a rate limiting OH addition Hydrated electrons were found to react with the 5-nitrouracils with rate consts. of 1.9 ± 0.2 + 1010M-1 sec-1 to produce the corresponding nitro anion radicals, which have been identified by their ESR spectra.
IT **17687-24-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(radiolysis of, oxidative denitration by hydroxyl radicals in)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



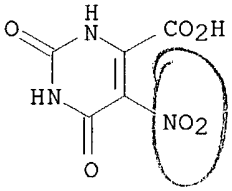
L6 ANSWER 104 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:166956 CAPLUS
DN 78:166956
TI Free radicals in irradiated nitro-substituted pyrimidines
AU Lorenz, Patrick; Benson, Brent
CS Dep. Phys., South. Illinois Univ., Carbondale, IL, USA
SO Radiation Research (1973), 53(3), 358-65
CODEN: RAREAE; ISSN: 0033-7587
DT Journal
LA English
AB X-irradiated 5-nitrobarbituric acid, 5-nitroorotic acid, and 5-nitro-4,6-dihydroxyprimidine show distinctive ESR spectra with very anisotropic N coupling, essentially the same as 5-nitrouracil. The 5-nitrouracil radical was identified as an iminoxyl radical formed by a mechanism which abstracts an O from the NO2 group leaving the unpaired electron coupling to the N of the NO2 group. These other nitropyrimidines yield similar iminozyl radicals. The only reported nitropyrimidine which yields different radical structures is 5-nitro-6-methyluracil which was investigated at 77 and 300°K by other workers. On the basis of these exptl. data, INDO (intermediate neglect of differential overlap) mol. orbital calcns., and the proposed mechanism of formation of the 5-nitrouracil which fits also the other nitropyrimidines radical structures for the low temperature and room temperature 5-nitro-6-methyluracil radicals can now be proposed. The proposed 77°K radical is formed by H addition to a nitro-oxygen leaving the unpaired electron coupling to this H and to the nitro-nitrogen. At room temperature the OH is abstracted from the NO2 group leaving it a NO group, and a H is added to O. INDO calcns. on this structure give very good agreement with the reported exptl. parameters. This radical is formed from the previously reported structure by alteration of the NO2 group into a NO group.
IT **17687-24-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(radiolysis of, by x-rays, ESR of iminoxy radicals from)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 107 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:25755 CAPLUS
DN 78:25755
TI Properties of a pyrimidine phosphoribosyltransferase from murine leukemia cells
AU Kessel, David; Deacon, Judith; Coffey, Barbara; Bekamjian, Ann
CS Sch. Med. Dent., Univ. Rochester, Rochester, NY, USA
SO Molecular Pharmacology (1972), 8(6), 731-9
CODEN: MOPMA3; ISSN: 0026-895X
DT Journal
LA English
AB A pyrimidine phosphoribosyltransferase (.apprx.100,000 mol. weight) with a sharply defined specificity was partially purified from ascitic cells of the P388/38280 murine leukemia. This enzyme is involved in the conversion of the antineoplastic drug 5-fluorouracil (Km = 100μM) to pharmacol. active nucleotides. The lowest Km value was obtained with orotic acid as substrate (Km = 50μM). The enzyme could also utilize 5-fluoroorotate (Km = 85μM) and uracil (Km = 5mM). Inhibition studies, using fluorouracil as substrate, indicate that this enzyme has a strong affinity for pyrimidines with a CO2H or NH2 group at position 6, or a F (but not a larger halogen) at position 5. A Me group at position 5 markedly decreases affinity of the enzyme for all pyrimidines. The affinity of the enzyme for 6-carboxypyrimidines was greatly increased in the presence of dimethyl sulfoxide, but the rate of the enzyme-catalyzed reaction was markedly decreased. The enzyme requires Mg2+ and phosphoribosyl pyrophosphate; the latter promotes stability at all temps. Enzyme extracted from a cell line made resistant to fluorouracil showed a decreased capacity to utilize fluorouracil as a substrate.
IT **7164-43-4 17687-24-0**
RL: BIOL (Biological study)
(orotate phosphoribosyltransferase inhibition by, kinetics of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



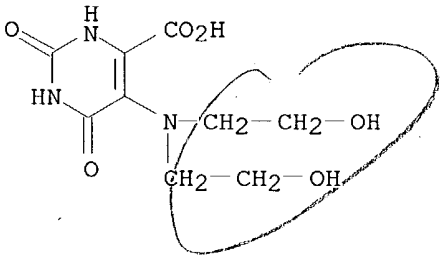
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 108 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:514343 CAPLUS
DN 77:114343
TI Pyrimidine derivatives. VI. Syntheses of orotic acid, uracil, and pyrimido[5,4-d]pyrimidine derivatives
AU Okui, Kiyoshi; Mizoguchi, Masakazu
CS Res. Lab., Chugai Pharm. Co., Ltd., Tokyo, Japan
SO Yakugaku Zasshi (1972), 92(7), 785-95
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
AB 5-Chloroorotic acid (I) was prepared via the intermediate II (obtained by the treatment of Et orotate with pyridine and thionyl chloride). 5-Chlorouracil and 5-chloromethylthiouracil were formed resp. by a similar reaction of uracil and methylthiouracil. The reaction is electrophilic with the thionylpyridinium chloride complex. An electron releasing group at the 4-position tends to lower the yield of 5-chloro compound, but an electron-withdrawing group gives a higher yield of 5-chloro compound The reaction of I or II with amine bases gave their substituted compds., in which substituents at the 4- and 5-positions did not lie coplanar to the pyrimidine ring. Treatment of the guanidine derivative (III) with concentrated H2SO4 gave the pyrimido-[5,4-d]pyrimidine derivative (IV).
IT **38245-70-4P 38245-71-5P 38245-72-6P**
38277-69-9P 38277-70-2P 38350-04-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38245-70-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[bis(2-hydroxyethyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, monohydrochloride, compd. with 2,2'-iminobis[ethanol] (1:1) (9CI) (CA INDEX NAME)

CM 1

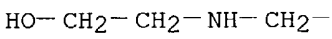
CRN 46863-45-0
CMF C9 H13 N3 O6 . Cl H



● HCl

CM 2

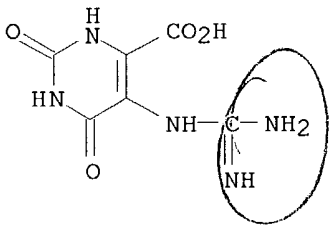
CRN 111-42-2
CMF C4 H11 N O2



RN 38245-71-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(aminoiminomethyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, monohydrochloride, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

CM 1

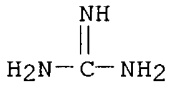
CRN 38350-04-8
CMF C6 H7 N5 O4 . Cl H



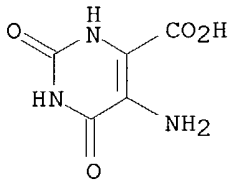
● HCl

CM 2

CRN 113-00-8
CMF C H5 N3



RN 38245-72-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, diammonium salt, monohydrochloride (9CI) (CA INDEX NAME)



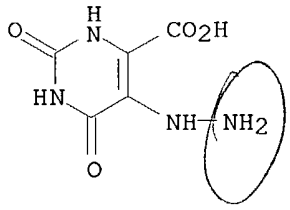
● HCl

● 2 NH_3

RN 38277-69-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-hydrazino-1,2,3,6-tetrahydro-2,6-dioxo-, compd. with hydrazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 46158-70-7
CMF C5 H6 N4 O4

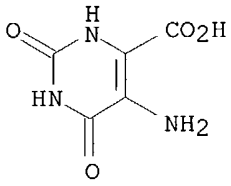


CM 2

CRN 302-01-2
CMF H4 N2

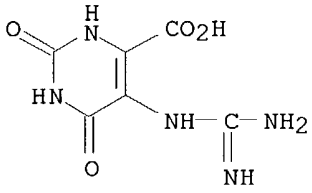
H_2N-NH_2

RN 38277-70-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)



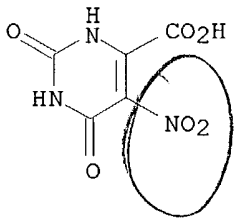
● HCl

RN 38350-04-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(aminoiminomethyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 109 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:494976 CAPLUS
DN 77:94976
TI Infrared spectra of pyrimidinecarboxylic acids, and problems of their structure
AU Titov, E. V.; Prikazchikova, L. P.; Rybchenko, L. I.; Cherkasov, V. M.; Rybachenko, V. I.
CS Donetsk. Inst. Fiz.-Org. Khim., Donetsk, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1972), (6), 833-5
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
AB The ir spectra of solid samples of 17 pyrimidinecarboxylic acids and of their solns. in dioxane and in CHCl3 were recorded. The frequencies of valence vibrations of CO2H groups, which did not participate in tautomerism were linearly correlated with acidity consts.: vCO = (1871 ± 7.5) - (40.6 ± 2.26) pKa.
IT **17687-24-0**
RL: PRP (Properties)
(ir spectrum of solid, structure in relation to)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



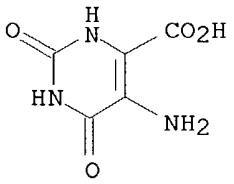
L6 ANSWER 110 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:488529 CAPLUS
DN 77:88529
TI 4,8-Bis(diethanolamino)--2,6-dipiperidinopyrimido[5,4-d]pyrimidine
IN Finotto, Martino
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2060640	A	19720615	DE 1970-2060640	19701209
PRAI	DE 1970-2060640		19701209		

AB The title compound (I), useful as a coronary blood vessel dilator, was prepared Chlorination of orotic acid with Cl gave 5-chloroorotic acid, treatment of which with NH4OH gave 5-aminoorotic acid (II). Reaction of II with urea gave homouric acid (III). Chlorination of the di-Na salt of III with POCl3 in DMF gave 2,4,6,8-tetrachloropyrimido[5,4-d]pyrimidine, which on reaction with piperidine gave 4,8-dichloro-2,6-dipiperidino-pyrimido[5,4-d]pyrimidine. Its treatment with NH3 in MeOH and, after addition of AcOH, with ethylene oxide gave I.

IT **7164-43-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



as before

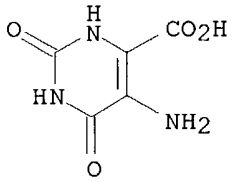
L6 ANSWER 111 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:153768 CAPLUS
DN 76:153768
TI 2,6-Bis(diethanolamino)-4,8-dipiperidinopyrimido[5,4-d]pyrimidine
IN Finotto, Martino
SO S. African, 17 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI ZA 7008332		19710803	ZA 1970-8332	19701209
FR 2117719			FR	

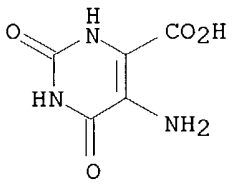
AB The title compound (I) was prepared from orotic acid by conversion into the 5-Cl and then the 5-NH2 derivative, which was treated with urea in an oil bath at 180°, then 230-240°, and then with HCl to give oxy-omuric acid (II); II with POCl3 and DMF gave the tetra-Cl analog, which with piperidine in anhydrous EtOH at room temperature gave I.

IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. with urea)

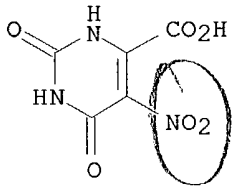
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



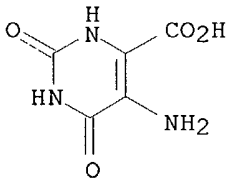
L6 ANSWER 112 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:153716 CAPLUS
DN 76:153716
TI Synthesis of some new products derived from pyrimido(5,4-d)pyrimidine
AU Gostea, T.; Gidea, Gabriela; Maza, Aurelia
CS Rom.
SO Revistade Chimie (Bucharest, Romania) (1971), 22(8), 468-70
CODEN: RCBUAU; ISSN: 0034-7752
DT Journal
LA Romanian
AB By heating 2,6-dichloro-4,8-bis(diethanolamino)pyr-imido[5,4-d]pyrimidine (I) with 2-, 3-, or 4-aminomethylpyridine 1 hr at 200°, the following II were obtained (R1, and % yield given): 2-pyridyl, 73.4; 3-pyridyl, 44; 4-pyridyl, 44. The following III (R1 and % yield given): 2-pyridyl, 35; 3-pyridyl, 43.5; 4-pyridyl, 29; were similarly prepared from IV.
IT **7164-43-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization with urea)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **17687-24-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

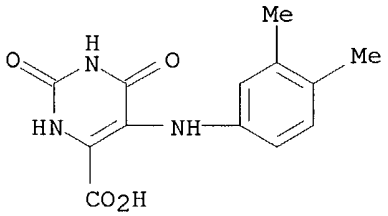


L6 ANSWER 113 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:95158 CAPLUS
DN 76:95158
TI Mutagenic effects of new purine and pyrimidine analogs on phage T4
AU Alikhanyan, S. I.; Piruzyan, E. S.; Mugnetsyan, E. G.
CS Inst. Genet. Sel. Ind. Microorg., Moscow, USSR
SO Mutation Research (1972), 14(1), 1-11
CODEN: MUREAV; ISSN: 0027-5107
DT Journal
LA English
AB Of 12 purine analogs tested, only 6-chloropurine [87-42-3] was mutagenic and only 6-mercaptopurine [50-44-2] was inactivating toward bacteriophage T4 growing on Escherichia coli. 6-Chloro-9-methylpurine (I) [2346-74-9] was not mutagenic, indicating that Me in the position 9 removes the mutagenicity of pyrimidine analogs. Among the 24 pyrimidine analogs tested, 2-amino-5-chloropyrimidine [5428-89-7] had twice the mutagenic activity as did 5-bromouracil (II) [51-20-7], and 2-aminopyrimidine [109-12-6], 2-amino-4-oxo-6-methylpyrimidine [3977-29-5], 5-(2-bromoethyl)-6-methyluracil [29622-40-0], and 2-amino-4-chloro-6-methylpyrimidine [5600-21-5] were as mutagenic as II. These analogs exist in tautomeric forms conducive to pairing with purine rings. 5-Bromoorotic acid (III) [15018-62-9], 5-aminoorotic acid [**7164-43-4**], 2-methylorotic acid [34415-10-6], and 2-aminoorotic acid [6973-52-0] were also mutagenic. The other pyrimidine analogs were inactive.
IT **7164-43-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mutagenic activity of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



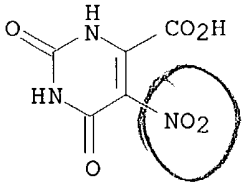
same as before

L6 ANSWER 114 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:85776 CAPLUS
DN 76:85776
TI Pyrimodo[5,4-b]quinolines. I. Synthesis of substituted tricyclic systems related to riboflavine
AU Levine, Edward M.; Bardos, Thomas J.
CS Sch. Pharm., State Univ. New York, Buffalo, NY, USA
SO Journal of Heterocyclic Chemistry (1972), 9(1), 91-7
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 76:85776
AB Two alternative synthetic routes were investigated for the synthesis of 2,4,10-substituted-7,8-dimethylpyrimido[5,4-b]-quinolines: (1) cyclization of 5-(3,4-xylidino)-2,4-disubstituted-pyrimidine-6-carboxylic acids, and (2) cyclization of N-5-(2,4-disubstituted-pyrimidinyl)-4,5-dimethylanthranilic acids. Route (1) invariably gave isomeric mixts. of the corresponding 7,8- and 8,9-dimethylpyrimido[5,4-b]quinolines which were difficult to sep., while route (2) yielded only the desired 7,8-dimethyl derivs. The required intermediates were synthesized by Ullmann-type condensation of the appropriate pyrimidine and benzene derivs. Cyclization with polyphosphoric acid, or POCl3 (under various conditions) gave new pyrimido[5,4-b]quinoline derivs., with oxo, methoxy and (or) chloro substituents in the 2,4 and 10 positions. A mild, but effective chlorination procedure was developed for the chlorination of the 10-(oxo) position without the cleavage of methoxyl groups at positions 2 and 4.
IT **35157-71-2**
RL: PROC (Process)
(preparation of)
RN 35157-71-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3,4-dimethylphenyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

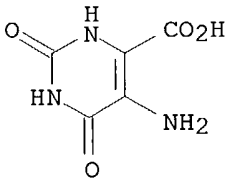


Sgutt Jnt

L6 ANSWER 115 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:20671 CAPLUS
DN 76:20671
TI Polarography of 5-nitroorotic acid
AU Gupta, S. L.; Kishore, N.; Raghavan, P. S.
CS Chem. Dep., Birla Inst. Technol. Sci., Pilani, India
SO Electrochimica Acta (1971), 16(12), 2135-9
CODEN: ELCAAV; ISSN: 0013-4686
DT Journal
LA English
AB The polarog. of 5-nitroorotic acid in aqueous medium was carried out at pH 1-10, using different buffer systems. There are 2 well-defined steps up to pH 9.0; the 1st step is purely diffusion-controlled (6e) reduction at all pH, and the 2nd step (4e) is purely diffusion-controlled in the acidic range and shows adsorption characteristics in the alkaline range. Above pH 9, the compound is reduced in 3 steps: the 1st is purely diffusion-controlled (4e); the 2nd (4e) and 3rd (2e) steps have adsorption character. At pH >11, the reduction involves 3 steps, but the wave heights are not reproducible. The number of electrons involved in the diffusion-controlled steps was determined by comparing the wave heights with that of the 1st step of PhNO2 reduction under identical conditions, which was confirmed by finding the diffusion coefficient D by using the McBain-Dowson cell. Kinetic parameters were computed for the diffusion-controlled steps by using Koutecky's method. The probable reduction mechanism is discussed.
IT **17687-24-0**
RL: PROC (Process)
(polarography of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

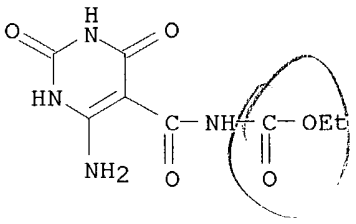


L6 ANSWER 116 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:73163 CAPLUS
DN 74:73163
TI Mutagenic and inactivating effects of pyrimidine derivatives on amber-mutants of bacteriophage T4
AU Mugnetsyan, E. G.; Piruzyan, E. S.; Alikhanyan, S. I.
CS State Univ., Erevan, USSR
SO Genetika (Moscow) (1970), 6(12), 93-100
CODEN: GNKAA5; ISSN: 0016-6758
DT Journal
LA Russian
AB 5-Bromouracil (I) and 5-bromodeoxyuridine induced reversions in phage T4 amber mutants B22 and A455 and caused transitions in both directions. Among 21 other pyrimidine derivs. studied, those carrying a labile H atom at positions 2,4, and 6 or a halogen atom at position 5 in the purine ring and existing in several tautomeric forms capable of pairing with a purine ring, exhibited mutagenic activity. These included 2-aminopyrimidine, 2-amino-5-chloropyrimidine, 2-amino-4-hydroxymethylpyrimidine, 5-β-bromoethyl-6-methyluracil, and 2-amino-4-chloro-6-methylpyrimidine. 5-Bromoorotic acid, 5-aminoorotic acid, and 2-methylorotic acid also induced reversion in the amber mutants B22 and A455.
IT **7164-43-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mutagenic activity of, to bacteriophage T4)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

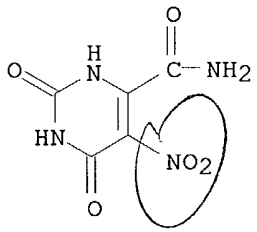


Same as boxed

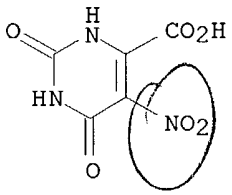
L6 ANSWER 117 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1970:100647 CAPLUS
DN 72:100647
TI New synthesis of the pyrimido[4,5-d]pyrimidine ring. Preparation of pyrimido[4,5-d]pyrimidine-2,4,5,7-tetrone
AU Niess, Rolf; Robins, Roland K.
CS Dep. of Chem., Univ. of Utah, Salt Lake City, UT, USA
SO Journal of Heterocyclic Chemistry (1970), 7(1), 243-4
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
AB The reaction of 1,3-di(R-substituted)-6-aminouracil with OCNCO2Et gave 1,3-di(R-substituted)-6-amino-5-[N-(carbethoxy)carboxamido]uracil, which upon heating gave 1,3-di(R-substituted)pyrimido[4,5-d]pyrimidine-2,4,5,7-tetrone (I, R = H). Similarly prepared was I (R = Me).
IT **26212-09-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26212-09-9 CAPLUS
CN Carbamic acid, [(6-amino-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)carbonyl]-, ethyl ester (8CI) (CA INDEX NAME)



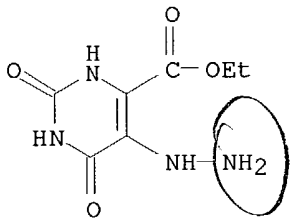
L6 ANSWER 118 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1970:31740 CAPLUS
DN 72:31740
TI Heterocyclic studies. XII. Trichloro-6-cyanopyrimidine
AU Clark, Jim; Pendergast, W.
CS Dep. Chem. and Appl. Chem., Univ. Salford, Salford, UK
SO Journal of the Chemical Society [Section] C: Organic (1969), (19), 2780-3
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
AB Treatment of 4-carbamoyl-2,6-dihydroxy-5-nitropyrimidine (I) with phosphoryl chloride and diethylaniline unexpectedly yielded 2,4,5-trichloro-6-cyanopyrimidine (II), together with 4-carbamoyl-2,6-dichloro-5-nitropyrimidine and a little 2-chloro-4-cyano-6-(N-ethylanilino)-5-nitropyrimidine. Some II was also obtained by treatment of I with phosphoryl chloride in the presence of dimethylaniline, pyridine, Et3N or PCl5. Nucleophilic substitution reactions of II, in which the cyano group was often displaced first, or modified, are described.
IT **19796-67-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19796-67-9 CAPLUS
CN Orotamide, 5-nitro- (8CI) (CA INDEX NAME)



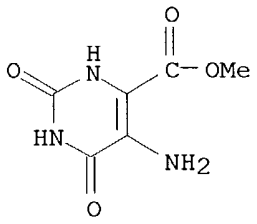
L6 ANSWER 119 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:508425 CAPLUS
DN 71:108425
TI 5-Nitro orotic acid. III. Electrochemical mechanism for the polarographic reduction of some nitro-pyrimidines
AU Jain, Padam C.; Kapoor, Ramesh C.
CS Univ. Jodhpur, Jodhpur, India
SO Journal of the Polarographic Society (1968), 14(4), 145-6
CODEN: JPLSA9; ISSN: 0554-4742
DT Journal
LA English
AB Polarographic behavior of 5-nitroorotic acid (I) was examined in aqueous medium using Britton-Robinson buffer at pH 7 and above. At pH 7, 8, and 9, I gave a well defined cathodic wave but at pH 10 the wave split into 2. The reduction process was irreversible and was not controlled by diffusion.
IT **17687-24-0**
RL: PROC (Process)
(polarography of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



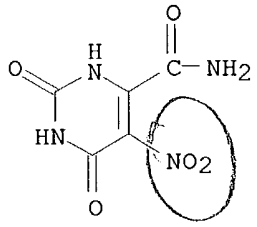
L6 ANSWER 120 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:422101 CAPLUS
DN 71:22101
TI Heteroaromaticity. XXVIII. Synthesis of pyrimidine derivatives
AU Sasaki, Tadashi; Ando, Moriyasu
CS Nagoya Univ., Nagoya, Japan
SO Yuki Gosei Kagaku Kyokaishi (1969), 27(2), 169-73
CODEN: YGKKAE; ISSN: 0037-9980
DT Journal
LA Japanese
AB Et 5-bromoorotate (0.1 g.) is refluxed in 20 ml. EtOH solution of 0.1 ml. 80% N2H4.H2O to give 0.04 g. Et 5-hydrazinoorotate, m. 237-9° (aqueous EtOH). Similarly prepared is Et 5-hydrazinouracil 6-acetate, m. 274-6°. An attempt to cyclize orotaldehyde hydrazone in AcOH failed, giving only orotaldehyde acetylhydrazone, m. >300° as the sole product. Uracil-6-acetic hydrazide (I), m. >300°, is synthesized almost quant. by heating Me or Et uracil 6-acetate in an EtOH solution of N2H4.H2O. I (0.85 g.) in 6 ml. H2O is treated with 2 ml. 10% HCl and 2 ml. aqueous solution of 0.4 g. KOCN to give 0.95 g. N1-(5-uracilacetic acid) semicarbazide (II), m. >300° (H2O). II (0.5 g.) warmed in 10% KOH gave 0.3 g. 2,4-dioxopyrimidino[5,6-d]-dihydropyridazin-3-one (III), m. >300°. Heating 0.6 g. I in 10 ml. MeOH with 0.5 ml. concentration HCl and 0.4 g. KSCN in 2 ml. H2O gives 0.56 g. bishydrazide IV, m. >300°. Treatment of 0.35 g. I with 0.4 ml. Ph isothiocyanate in 10 ml. pyridine 5 hrs. gives 0.4 g. N1-(uracil-5-acetyl)-N4-phenylthiosemicarbazide (V), m. 243-4° (aqueous EtOH). Heating 0.1 g. V in 10 ml. 10% NaOH at 85° 2 hrs. gives 0.06 g. VI, m. >300° (aqueous EtOH). Reactions of 0.2 g. I with 1 ml. CS2 and with 0.5 ml. Et acetoacetate give 0.12 g. II and VII, m. 180-4° (EtOH), resp.
IT **23090-84-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23090-84-8 CAPLUS
CN Orotic acid, 5-hydrazino-, ethyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 121 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:467339 CAPLUS
DN 69:67339
TI Pteridines. X. Some pyrimidopyrimidine isomers of triamterene
AU Graboyes, Harold; Jaffe, Gerald E.; Pachter, Irwin J.; Rosenbloom, Joanne P.; Villani, Anthony J.; Wilson, James W.; Weinstock, Joseph
CS Res. and Develop. Div., Smith Kline and French Lab., Philadelphia, PA, USA
SO Journal of Medicinal Chemistry (1968), 11(3), 568-73
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB 2,4,7-Triamino-5-phenylpyrimido[4,5-d]pyrimidine was prepared by the condensation of guanidine with 2,6-diamino-5-cyano-4-phenylpyrimidine. Similar reactions gave 5-alkyl analogs of this compound An attempt to use 4-amino-5-cyano-2,6-dimethylpyrimidine in this reaction gave 2,4,7-triamino-5-methylpyrimido[4,5-d]pyrimidine in contrast to the diphenyl analog which gave the expected product. 2,4,5-Triamino-7-phenylpyrimido[4,5-d]pyrimidine was prepared by the fusion of guanidine carbonate with 4-amino-5-cyano-6-(methylthio)-2-phenylpyrimidine. 2,4,8-Triamino-6-phenylpyrimido[5,4-d]pyrimidine was prepared by condensation of Me 2,4,5-triaminopyrimidine-6-carboxylate with benzamidine to form 2,4-diamino-8-hydroxy-6-phenylpyrimido[5,4-d]pyrimidine followed by deoxychlorination and amination. 18 references.
IT **19796-65-7P 19796-66-8P 19796-67-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19796-65-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)

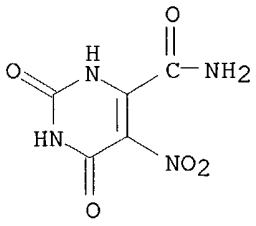


RN 19796-66-8 CAPLUS
CN Orotamide, 5-nitro-, monoammonium salt (8CI) (CA INDEX NAME)

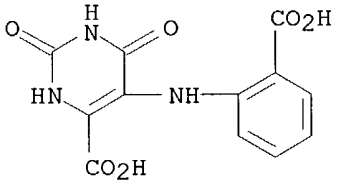


● NH_3

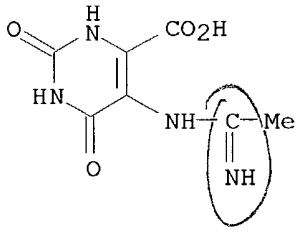
RN 19796-67-9 CAPLUS
CN Orotamide, 5-nitro- (8CI) (CA INDEX NAME)



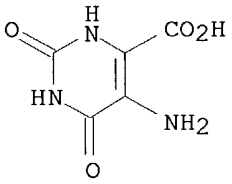
L6 ANSWER 122 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:459179 CAPLUS
DN 69:59179
TI Substituted heteroaromatic anthranilic acids with antiinflammatory activity
AU Falch, E.; Weis, J.; Natvig, T.
CS Res. Div., Pharmacia AS, Copenhagen-Vanloese, Den.
SO Journal of Medicinal Chemistry (1968), 11(3), 608-11
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Anthranilic acids (I and II) containing heteroaromatic N-substituents were prepared by the reaction of appropriately substituted chloro heterocycles with anthranilic acid in HCl or substituted methylthio heterocycles with anthranilic acid in alkaline solution The reaction of o-BrC6H4CO2H with 5-amino-4-carboxy-2,6-dihydroxypyrimidine gave N-[5-(4-carboxy-2,6-dihydroxypyrimidinyl)]anthranilic acid. The exchange of the o-xylyl moiety in mefenamic acid with heteroaromatic rings significantly lowers the antinflammatory activity.
IT **19573-76-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19573-76-3 CAPLUS
CN Orotic acid, 5-(o-carboxyanilino)- (8CI) (CA INDEX NAME)



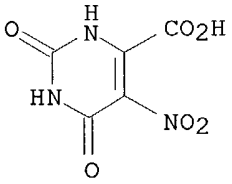
L6 ANSWER 123 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:508627 CAPLUS
DN 67:108627
TI Reactions with imido acid esters. IX. Quinazolones, azaquinazolones, and amidines from imidic acid esters and aromatic amino carboxylic acids
AU Ried, Walter; Valentin, Joachim
CS Univ. Frankfurt/M., Frankfurt/M., Fed. Rep. Ger.
SO Justus Liebigs Annalen der Chemie (1967), 707, 250-5
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA German
OS CASREACT 67:108627
AB cf. CA 67: 108543b. Imidocarboxylic acid esters reacted with substituted anthranilic acids to give substituted quinazol-4-ones. The highest yield (47%) was shown by the reaction between 2,4-(H2N)2C6H3CO2H and MeC(:NH)OH esters giving 2-methyl-7-aminoquinazol-4-one. Similarly, aminopyridinecarboxylic acids gave pyridopyrimidones. Thus, the reaction between 3-aminopyridine-4-carboxylic acid and MeC(:NH)OH esters yielded 2-methylpyrido[3,4-d]pyrimidin-4-one (I). The reaction of MeC(:NH)OH esters with aminoorotic acid yielded N-(2,4-dihydroxy-6-carboxypyrimidin-5-yl)acetamidine betaine (II).
IT **16081-88-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16081-88-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetimidoylamino)-2,6-dihydroxy- (8CI) (CA INDEX NAME)



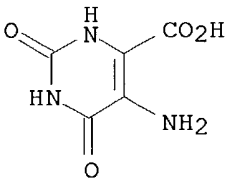
L6 ANSWER 124 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:476706 CAPLUS
DN 67:76706
TI Linear free energy relations for proton dissociation and metal complexation of pyrimidine acids
AU Tucci, Edmond R.; Ke, Charles H.; Li, Norman C.
CS Duquesne Univ., Pittsburg, PA, USA
SO Journal of Inorganic and Nuclear Chemistry (1967), 29(7), 1657-67
CODEN: JINCAO; ISSN: 0022-1902
DT Journal
LA English
AB Linear free energy relations for proton dissociation and metal complexation were investigated for the pyrimidine acid system. Linear correlations were obtained when pKa20' - pKa2' values for 5-substituted uracil carboxylic acids were plotted against the Hammett substituent constants, σm. The large calculated ρ value of 5.78 indicates that the 2nd proton dissociation for this acid series is very sensitive to substituent effects. Calculated "effective" substituent consts. (σm) for these pyrimidine acids are in reasonable agreement with the Hammett σm values. With the exception of 5-nitroorotic acid, a fair linear correlation was obtained in plotting σm or pKa2' vs. log KMA for 5-substituted uracil-6-carboxylic (orotic) acid complexes of Ni(II), Co(II), Zn(II), and Cd(II). Abnormally high log KMA values for 5-nitroorotic acid, as compared with ligand basicity, were partly attributed to πelectron backdonation by the metal ion to the ligand. In plots of log KZnA vs. log KM'A, where M' is Co(II), Ni(II), or Cd(II) and A is a 5-substituted orotic acid, linear correlations were observed with unit slopes. That linear correlations are best observed by comparing structurally similar ligands with identical reaction sites was illustrated by plotting log KMA for isoorotic acid vs. log KMA for 2-ethylthioisoorotic acid, or orotic acid. A good linear correlation was observed between isoorotic acid and 2-ethyl thioisoorotic acid complexes, but no linear correlation was observed between isoorotic acid and orotic acid complexes.
IT **7164-43-4 17687-24-0**
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(ionization of, substituent constant and)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



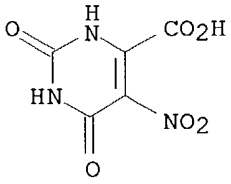
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



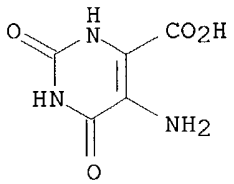
L6 ANSWER 125 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:469036 CAPLUS
DN 67:69036
TI Infrared spectra of some derivatives of pyrimidine-carboxylic acid
AU Hermann, Theodore S.; Black, J. M.
CS Midwest Res. Inst., Kansas City, MO, USA
SO Applied Spectroscopy (1966), 20(6), 413-14
CODEN: APSPA4; ISSN: 0003-7028
DT Journal
LA English
AB cf. Short and Thompson, CA 46: 9986e; Lord, et al., CA 51: 14423d. The KBr disk ir spectra of 36 pyrimidine-4-carboxylic acids substituted in the 2- and 6-positions with hydroxy, mercapto, or amino (Daves, et al., CA 55: 27343b) have been studied. The pyrimidine ring vibrations are tabulated and the ranges of frequencies assigned to the ring modes are 1655-1565, 1470-1390, 1000-940, and 725-680 cm.-1
IT **7164-43-4 17687-24-0**
RL: PRP (Properties)
(spectrum (ir) of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



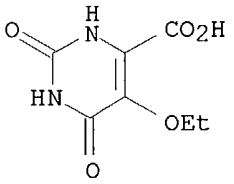
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



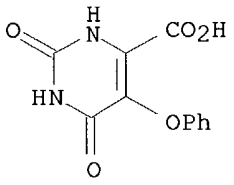
L6 ANSWER 126 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:16228 CAPLUS
DN 66:16228
TI Derivatives of orotic acid as potential reagents for the alkali metals
AU Lewis, B. C.; Stephen, William I.
CS Univ. Birmingham, Birmingham, UK
SO Analytica Chimica Acta (1966), 36(2), 234-7
CODEN: ACACAM; ISSN: 0003-2670
DT Journal
LA English
AB The reactions were examined of the alkali metal ions with orotic acid (2,6-dihydroxypyrimidine-4-carboxylic acid) (I), with 18 N-and C-5-substituted derivs. of I, uracil-5-carboxylic acid (II), and with 5 derivs. and analogs of II, used in the form of their N,N-dimethylethanolammonium salts (III) (0.1M in 80% Et-OH). The III salts of the reagents were prepared in the manner described by Selleri and Caldini (CA 56, 7994b). The solubilities of the alkali metal salts of various pyrimidinecarboxylic acids (I, II, and their derivs.) were determined in H2O, 80% aqueous-EtOH, and in 90% EtOH. To 1 ml. of the aqueous alkali metal Cl- solution, containing 10 mg. of the cation/ml., was added 5 ml. of 0.1M reagent (in 80% EtOH). The solution was mixed and examined for formation of a precipitate To 40 ml. of 0.1M reagent (in EtOH) was added 10 ml. of 5% aq alkali metal Cl- solution The ppts. were aged for several hrs. at 3°, filtered on sintered glass crucibles, washed with 4-5 2-ml. vols. of 70% EtOH, and 2 2-ml. vols. of 95% EtOH, and dired at 105° for 1 hr. In every case, the precipitate was the normal salt. Few of the compds. show a useful degree of selectivity or sensitivity. Uracil-3-acetic acid gives a selective reaction with Li+; 5-ethyl derivative of I with Na+; and 5-methyluracil-3-acetic acid (IV) with K+; IV easily distinguishes between K+ and Rb+. Precipitation of Li+, Na+, and K+ with the latter 3 reagents, resp., occurs only in solns. containing .apprx.90% EtOH. None of the I derivs. is as sensitive as I toward the alkali metals; substitution in I usually resulted in increased solubility of the corresponding alkali metal salts. The solubility values (g./l.) of the Li+, Na+, K+, Rb+, and Cs+ salts, resp., in H2O, 80% EtOH, and 90% EtOH at 25° are: I -, 1.08, 0.33; 2.94, 0.08, 0.03; 2.57, 0.07, 0.03; 5.59, 0.21, 0.15; 30.82, 1.55, 0.22; II -, 0.54, 0.19; -, 0.08, 0.03; -, 0.14, 0.06; -, 0.32, 0.08; -, 0.63, 0.21; (5-methyl derivative of I) -, -, -; -, 0.91, 0.26; -, 1.57, 0.78; -, 3.47, 1.41; -, 2.81, 0.85 g./l., resp.
IT **7164-43-4 14383-30-3 14383-34-7 14383-37-0 14383-38-1 17687-24-0**
RL: ANST (Analytical study)
(in alkali metal determination)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



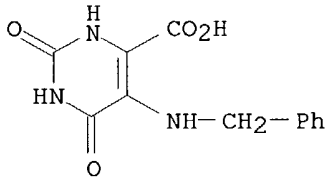
RN 14383-30-3 CAPLUS
CN Orotic acid, 5-ethoxy- (8CI) (CA INDEX NAME)



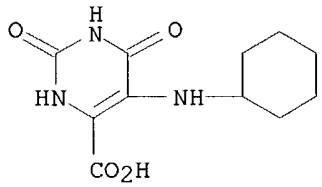
RN 14383-34-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-phenoxy- (9CI) (CA INDEX NAME)



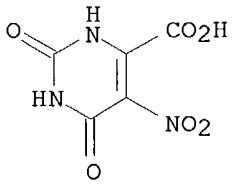
RN 14383-37-0 CAPLUS
CN Orotic acid, 5-(benzylamino)- (8CI) (CA INDEX NAME)



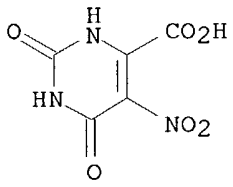
RN 14383-38-1 CAPLUS
CN Orotic acid, 5-(cyclohexylamino)- (8CI) (CA INDEX NAME)



RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 127 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:100955 CAPLUS
DN 64:100955
OREF 64:18935f-h,18936a
TI Metal complexes of pyrimidine derivatives and adenosine monophosphate. III
AU Doody, Br. E.; Tucci, E. R.; Scruggs, R.; Li, N. C.
CS Christian Brothers Coll., Memphis, TN
SO Journal of Inorganic and Nuclear Chemistry (1966), 28(3), 833-44
CODEN: JINCAO; ISSN: 0022-1902
DT Journal
LA English
AB cf. CA 56, 2035g. The following compds. were investigated by ion-exchange or potentiometric methods for complex formation in the presence of bivalent metal ions: uracil-5-carboxylic acid, uracil-6-carboxylic acid, 5-nitroorotic acid, 2-ethylthioisoorotic acid, 2-thioisoorotic acid, adenosine-3'-phosphate (3'-AMP), adenosine-5'-phosphate (5'-AMP), and α-D-glucose-1'-phosphate (1'-GP). Radiochem. cation-exchange expts. indicated no complexing of Zn(II) ions with uracil-6-carboxylic acid, while mononuclear species were found for the remaining pyrimidine complexes of Zn(II), Co(II), and Mn(II), in the pH range studied. Formation consts. calculated by cation-exchange methods were in good agreement with titration values. Potentiometric studies of adenosine-3'-phosphate indicated that the predominant species was the normal mononuclear complex (MA), but that the existence of a protonated complex (MHA) does exist. Equilibrium consts. were calculated for MHA complexes of 3'-AMP and Ni(II), Co(II), and Mn(II) ions: formation consts. were determined for MA complexes of Zn(II), Co(II), and Mn(II) by using ion-exchange and titration methods. For 3'-AMP, the stability of the MA complex followed the order, Zn > Co > Mn. Formation consts. calculated for the MA mononuclear 5'-AMP complexes indicated the trend in complex stability, Ni > Co > Mn. An iterative computer program was written for normal and protonated complexes for dibasic acids and divalent metal ions. Complexation studies of α-D-glucose-1'-phosphate supported the view that the adenosine residue does not play a major role in metal complexing. Formation consts. were calculated for mononuclear 1'-GP complexes of Zn(II), Co(II), and Mn(II). The relative order of stability for Co(II), and Mn(II) complexes of the phosphate ligands studied was 5'-AMP > 1'-GP > 3'-AMP.
IT **17687-24-0**, Orotic acid, 5-nitro-
(complexes with Co and Mn)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

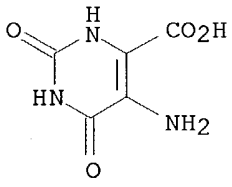


L6 ANSWER 128 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:11539 CAPLUS
DN 64:11539
OREF 64:2103h,2104a-b
TI 5-Aminoorotic acid
IN Goldner, Herbert; Trampau, Lothar
SO 2 pp.
DT Patent
LA Unavailable
FAN.CNT 1

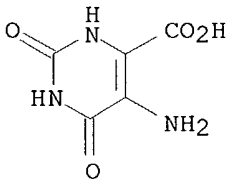
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 39698		19650615	DD	19641017

AB 5-Aminoorotic acid (5-aminouracil-4-carboxylic acid) (I) is made by oxidation of 4-methyl-5-nitrouracil (II) with HNO3 (d = 1.5) to obtain 5-nitrouracil-4-carboxylic acid (III) which is dissolved in water, neutralized with NaOH to pH 3-4, and reduced with Na2S2O4. Thus, 342 g. II was heated with 800 ml. fuming HNO3 (d = 1.5) to 70°. Then the exothermic reaction started and the temperature in the mixture rose to 100°. After the reaction was finished, the mixture was heated 1 hr. on a steam bath. Then the solid cake of III, remaining in the vessel was dissolved in 1.4 l. water, and the solution brought to pH 3-4 with NaOH until the Na salt of III precipitated This suspension was added to a cooled solution of 1.26 kg. Na2S2O4 in 4 l. water at 30°; 0.5 hrs. after the suspension had been added the mixture was tested if reducing agents were still present and it was acidified with 1.3 l. HCl. After 3 hrs. 273-91 g. 95% I was filtered off.

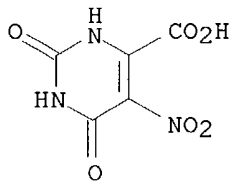
IT **7164-43-4**, Orotic acid, 5-amino-
(preparation of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



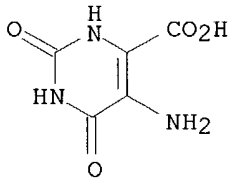
L6 ANSWER 129 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:433765 CAPLUS
DN 61:33765
OREF 61:5944c-f
TI Metal complexation with pyrimidine derivatives. III. 5-Substituted orotic acids
AU Tucci, E. R.; Takahashi, F.; Tucci, V. A.; Li, N. C.
CS Duquesne Univ., Pittsburgh, PA
SO Journal of Inorganic and Nuclear Chemistry (1964), 26(7), 1263-76
CODEN: JINCAO; ISSN: 0022-1902
DT Journal
LA Unavailable
AB cf. CA 58, 12151f. Metal complexes of the following uracil series of pyrimidine N bases were studied to assist in elucidating the effect of metal-irons on the double-stranded helical structure of nucleic acids: 5-bromouracil- 6-carboxylic acid (5-bromoorotic acid), 5-nitroorotic acid, 5-amino orotic acid, and 5-iodoorotic acid. Formation consts., calculated for bivalent metalion complexes, indicated that stable complexes were formed with these pyrimidine acids and the order of complex stability was: Cu(II) ≥ Ni(II) ≥ Co(II) ≥ Zn(II) Cd(II) ≥ Mn(II).
These metal ions were capable of removing the proton on the N1-pyrimidine ring-N, which is believed to be partly responsible for H bonding between the 2 helical ribose phosphate chains. The trend in complex stability for the ligands was similar to that observed for the basicity of the N1-pyrimidine ring-N, that is, 5-aminoorotic acid > 5-iodoorotic acid > 5-bromoorotic acid > 5-nitroorotic acid. The possible formation of protonic complexes was either negligible or completely absent in the pH region where one would normally expect to find these complexes. Only mononuclear complexation was observed. An equation was derived to determine formation consts. for 1:1 complexes of these pyrimidine acids from their ultraviolet light absorption spectra. These spectra, which were determined at various pH values in the absence or presence of metal ions, are briefly discussed.
IT **7164-43-4**, Orotic acid, 5-amino- **17687-24-0**, Orotic acid, 5-nitro-
(metal complexes)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



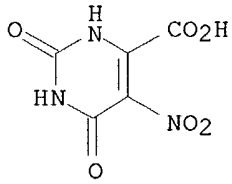
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



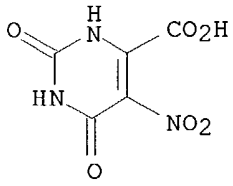
L6 ANSWER 130 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1963:471255 CAPLUS
DN 59:71255
OREF 59:13239f-g
TI Pattern of anticytogenic activity of pyrimidine derivatives on Neurospora crassa
AU Rauen, H. M.; Nonhof, R.
CS Univ. Muenster, Westfalen, Germany
SO Arzneimittel-Forschung (1963), 13(7), 558-66
CODEN: ARZNAD; ISSN: 0004-4172
DT Journal
LA Unavailable
AB The anticytogenic activity of 71 pyrimidine derivs. on N. crassa was determined in the horizontal proliferation test. Of these, the following 12 were found to meet the criteria of the Cancer Chemotherapy National Service Center; i.e., their inhibitory doses (H.D.50) were under the limit of 10 mg./ml. of culture medium: 2-ethylmercapto-4-chloro-5-carbethoxypyrimidine, 0.025; bis(4-methylpyrimidyl-2-disulfide, 0.044; 4,6-dichloropyrimidine, 0.060; 4-methylpyrimidyl-2-sulfenmorpholide, 0.086; 2-ethylmercapto-4-amino-4-carbethoxypyrimidine, 0.130; 2-ethylmercapto-4-hydroxycarbethoxypyrimidine, 0.85; 4-phenylpyrimidine ,0.200; 2,4,5,6-tetraaminopyrimidine sulfate, 0.350; 2-amino-4-chloro-6-methylpyrimidine, 0.370; 2,4-dimercaptopyrimidine, 0.400; 2-mercapto-4-methylpyrimidine-HCl, 0.500; 2-mercapto-4,6-dimethylpyrimidine, 0.550 mg. Combinations of 2 or more inhibitory materials showed additive, synergistic, or diminished effects. The possible inhibitory mechanism is discussed. Relations are shown between the structures of the compds. and their cytotoxic action.
IT **7164-43-4**, Orotic acid, 5-amino- **17687-24-0**, Orotic acid, 5-nitro-
(Neurospora crassa inhibition by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



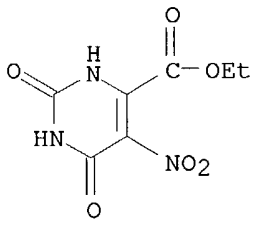
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



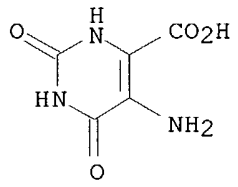
L6 ANSWER 131 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1963:71193 CAPLUS
DN 58:71193
OREF 58:12151f-h,12152a-d
TI Metal complexation with pyrimidine derivatives. II. Spectrophotometric studies
AU Tucci, Edmond R.; Li, Norman C.
CS Duquesne Univ., Pittsburgh, PA
SO Journal of Inorganic and Nuclear Chemistry (1963), 25, 17-27
CODEN: JINCAO; ISSN: 0022-1902
DT Journal
LA Unavailable
AB cf. CA 56, 2035g. Ultraviolet light absorption studies were made on a number of pyrimidine derivs. in H2O or D2O, both as a function of pH and in the absence or presence of metal ions. The pyrimidine compds. studied included: uracil-5-carboxylic acid (isoorotic acid), 2-ethylthioisoorotic acid, uracil-6-carboxylic acid (orotic acid), 5-nitroorotic acid, and their corresponding esters. Isoorotic acid was very pH sensitive in H2O and D2O. Identical spectral curves were obtained in both solvent systems. A lowering of the extinction coefficient at pH 6, as compared with pH 1, could indicate an ionization effect rather than enolization since no appreciable wavelength shift was observed. However, enolization is predominant in the region of pH 12. A confirmation that pK2 in isoorotic acid refers to proton dissociation from an enolic species was obtained by determining the pK2 of isoorotic acid in H2O and in D2O. In the presence of Cu(II) ions at pH 3, there was noted a slight shift towards the visible in the region of the uracil absorption band of isoorotic acid. This slight shift is attributed to complexing through the ketonic O and carboxyl group. Very little shift in the uracil lactam band occurred in going from the acidic to neutral region for orotic acid and a slight shift to longer wavelengths resulted when approaching the region of pH 12. Ultraviolet absorption spectra obtained in D2O indicated that even up to pH 12, orotic acid was still predominantly mono or diketonic. D isotope studies indicate at least one monoketonic form at pH 10. Spectral curves show that in the presence of Zn(II), Co(II), and Mn(II), orotic acid forms weak complexes. However, in the presence of Cu(II) and Ni(II) ions strong complexing is observed. A D isotope effect was noted with orotic acid and Ni(II) ions in D2O resulting from the cleavage of the D-N1 bond and verifying complexation through the carboxyl group and N in the 1-position. The nitro group in 5-nitroorotic acid appears to considerably modify the lactam-lactim equilibrium in the pyrimidine nucleus, favoring enolization in the neutral and high pH regions. 5-Nitroorotic acid complexes strongly with Cu(II) at pH 6, but is almost independent of Ni(II) ions. The ethylthio group in 2-ethylthioisoorotic acid appears to cause enhanced enolization of the carbonyl group in the 4-position. Complexing with Cu(II) ions is quite similar to isoorotic acid in magnitude.
IT **17687-24-0**, Orotic acid, 5-nitro-
(enolization, ionization and spectrum of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



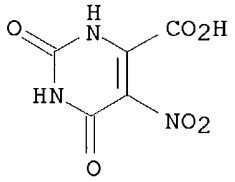
L6 ANSWER 132 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:435361 CAPLUS
DN 57:35361
OREF 57:7002d-g
TI Electrochemical characteristics of organic compounds. IX. Pyrimidine compounds
AU Glicksman, R.
CS Radio Corp. of Am., Somerville, NJ
SO Journal of the Electrochemical Society (1962), 109, 352-6
CODEN: JESOAN; ISSN: 0013-4651
DT Journal
LA Unavailable
AB cf. CA 56, 4505e. Half-cell potentials of substituted pyrimidines were studied with (a) nitropyrimidine compds. as cathodes in MgBr2 electrolyte, and (b) aminoand hydroxypyrimidines as anodes in NaOH electrolyte. Data are presented for the following group (a) compds.: 2-nitroresorcinol, 2,4-dichloronitrobenzene, 2,4-dichloro-5-nitropyrimidine, 4,6-dichloro-5-nitropyrimidine, 4,6-dihydroxy-5-nitropyrimidine, 2,4-dihydroxy-5-nitropyrimidine, 2,4-diamino-5-nitropyrimidine, 2,4-dihydroxy-5-nitro-6-carboxypyrimidine Et ester, 2,4,6-trihydroxy-5-nitropyrimidine, 2,4,6-trihydroxy-5-nitrosopyrimidine, 2,4,6-triamino5-nitrosopyrimidine; and for group (b) compds.: o-phenylenediamine, 4,5-diaminopyrimidine, p-phenylenediamine, 2,5-diaminopyrimidine, phloroglucinol, barbituric acid, cyanuric acid, resorcinol, uracil, 5-aminouracil, 6-aminouracil, 5-hydroxybarbituric acid, 5-aminobarbituric acid, 2,5-diamino-4,6-dihydroxypyrimidine, 2,4,5-triamino-6-hydroxypyrimidine sulfate, 2,5-diaminopyrimidine, 2,4,6-triaminopyrimidine, and melamine. Some of these are compared with the corresponding benzene compds. with regard to theoretical capacity and electrode efficiency. The potentials of the compds. are dependent on the aromaticity of the pyrimidine ring and on its substituents. This can be explained in terms of the electron-d, distribution of the mol.
IT **52047-16-2**, Orotic acid, 5-nitro-, ethyl ester
(potential of)
RN 52047-16-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 133 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:431342 CAPLUS
DN 57:31342
OREF 57:6307e-h
TI Properties of triphosphopyridine nucleotide-linked dihydroorotic dehydrogenase
AU Udaka, Shigezo; Vennesland, Birgit
CS Univ. of Chicago
SO Journal of Biological Chemistry (1962), 237, 2018-24
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA Unavailable
AB A procedure has been described for the partial purification of induced, triphosphopyridine nucleotide (TPN)-linked dihydroorotic dehydrogenase from an unidentified aerobic bacterium. The stoichiometry of the reaction catalyzed has been demonstrated, and the equilibrium constant has been determined The enzyme appears to be similar in many respect to the diphosphopyridine nucleotide (DPN)-linked dihydroorotic dehydrogenase previously purified from the anaerobe, Zymobacterium oroticium. Like the DPN-linked enzyme, the TPN-linked enzyme is a globulin flavoprotein. Throughout the later stages of the purification, the turnover number with respect to flavine was fairly constant at approx. 700 moles/mole of flavine/min. The flavine prosthetic group could be bleached by dihydroorotate and by TPNH, and preliminary evidence suggests that it probably consists of equal amts. of flavine mononucleotide and flavine adenine dinucleotide. The TPN-linked enzyme contains relatively trivial amts. of TPNH oxidase. Sulfhydryl groups are essential for activity but are much less sensitive than the SH groups of the DPN-linked enzyme. The bacteria are capable of growth on a simple medium containing inorg. salts and either orotate or aspartate as a source of C and N. 5-Fluoroorotate, which is an excellent substrate for the enzyme, inhibits growth on either orotate or aspartate. There are no appreciable changes in the flavine content of the bacterial cells during enzyme induction. Both 5-aminoorotate and 5-methylorotate cause appreciable enzyme induction when added to the aspartate medium, although neither of these orotate analogs supports growth.
IT **7164-43-4**, Orotic acid, 5-amino-
(dihydroorotate dehydrogenase induction by)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

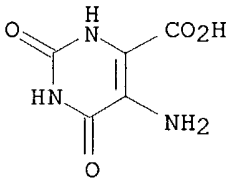


L6 ANSWER 134 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:10954 CAPLUS
DN 56:10954
OREF 56:2035g-i
TI Acid dissociation constants and complex formation constunts of several pyrimidine derivatives
AU Tucci, Edmond R.; Doody, Edward, Brother; Li, Norman C.
CS Duquesne Univ., Pittsburgh, PA
SO Journal of Physical Chemistry (1961), 65, 1570-4
CODEN: JPCHAX; ISSN: 0022-3654
DT Journal
LA Unavailable
AB Acid dissociation consts. of uracil-5-carboxylic acid (isoorotic acid) (I), were 2-ethylthioisoorotic acid (II), uracil-6-carboxylic acid (orotic acid) (III), 5-nitroorotic acid (IV), and adenosine-5'-monophosphate (V) were determined at an ionic strength of 0.1 and 25°. The formation constants of the Cu(II), Ni(II), Co(II), Zn(II), Mn(II), Cd(II) complexes of some of these pyrimidine derivs. were determined by pH and ion-exchange methods. The binding sites in I and II toward metal ions are probably the carboxylate anion and the adjacent O atom. The postulated sites in IV toward metal ions and toward Ni ion are the carboxylate and adjacent ring N anions. The formation consts. of the Zn complexes of I and IV, and of the Na and manganous complexes of V obtained by the pH method agree with the corresponding values obtained by the ion-exchange method, indicating that these complexes are mononuclear.
IT **17687-24-0**, Orotic acid, 5-nitro-
(ionization of)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)

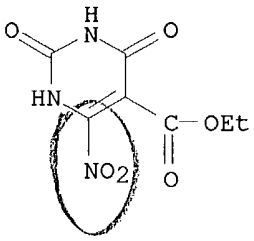


(metal complexes, ionization of

L6 ANSWER 135 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:33578 CAPLUS
DN 55:33578
OREF 55:6603c-e
TI Effect of some pyrimidine derivatives on the multiplication of tobacco mosaic virus
AU Ulrychova-Zelinkova, Marie
CS Czech. Acad. Sci., Prague
SO Biol. Plant. Acad. Sci. Bohemoslov. (1960), 2, 240-3
DT Journal
LA English
AB The effect of 17 pyrimidine derivs. was tested in leaf-disk cultures. The greatest antiviral effect was found with 2-amino-4-methyl-6-chloropyrimidine (I) which showed 98% inhibition at 500 γ/ml. and 50% at 50 γ/ml. The 6-hydroxy analog of I was about 75% as effective as I. Uracil and ethyl S-(4-methyl-6-hydroxy-2-pyrimidyl)thioglycolate at 500 γ/ml. stimulated viral production, whereas the following compds. were toxic at 500 γ/ml.: 2,6-dichloropyrimidine; 2,6-dichloro-4-methylpyrimidine; 2-thio-4,6-dihydroxypyrimidine, 2,4-dichloropyrimidine; 2,4,6-trichloropyrimidine; and 2,6-dichloro-4-trichloromethylpyrimidine. The following were weakly inhibitory or inert: 2-amino-2,6-dihydroxypyrimidine; 4-amino-2,6-dihydroxypyrimidine; 2,6-dihydroxy-4-methylpyrimidine; 2-thio-4-methyl-6-hydroxypyrimidine; 2,6-dihydroxy-4-carboxy-5-aminopyrimidine.
IT **7164-43-4**, 4-Pyrimidinecarboxylic acid, 5-amino-2,6-dihydroxy- (effect on tobacco mosaic virus)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 136 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:24604 CAPLUS
DN 55:24604
OREF 55:4861f-i
TI Some pyrimidine derivatives as new types of plant stimulants
AU Sormova, Z.; Melichar, O.; Sorm, F.
CS Ceskoslov. akad. ved, Prague
SO Collection of Czechoslovak Chemical Communications (1960), 25, 2889-98
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
AB Certain analogs of thymine and uracil revealed a stimulant effect on the development of plants. 5-Bromouracil and 5-cyanuracil accelerated only the development of the hypocotyl, while 2-thio-6-azauracil (I) and 2-thio-5-phenyl-6-azauracil (II) supported growth of the root system. Only a few compds. displayed a stimulating effect on the growth both of the epigeous and subterranean parts of the plant, of which 5-nitrouracil gave the most significant results, suggesting its application in agricultural practice. Similarly successful were I and II, since application in concns. of 50 γ/ml. brought about an increase in sugar content in sugar-beet by 1.05 and 0.25%, resp., with simultaneous decrease in the amount of harmful amide N and ash. The stimulation of plants was effected by very low concns. of the above compds., since penetration of 0.01-1.0 γ compound into 1 seed caused permanent developmental changes that were reflected, not only during the initial stages, but during the entire vegetation period of the plant. Morphological changes observed in cucumbers indicate a complex interference in the region of nucleic acid metabolism. Cytological expts. revealed that the above analogs of pyrimidine bases do not affect longitudinal growth but rather the mitotic activity of plant cells.
IT **100958-76-7**, 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-nitro-2,4-dioxo-, ethyl ester
(as plant regulator)
RN 100958-76-7 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-nitro-2,4-dioxo-, ethyl ester (6CI) (CA INDEX NAME)



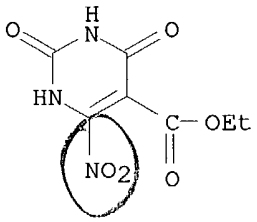
L6 ANSWER 137 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1960:23177 CAPLUS
DN 54:23177
OREF 54:4611a-i,4612a
TI Nucleic acid components and their analogs. III. Antimicrobial effect of some pyrimidine analogs and related compounds
AU Gut, J.; Moravek, J.; Parkanyi, C.; Prystas, M.; Skoda, J.; Sorm, F.
CS Ceskoslov. akad. ved, Prague
SO Collection of Czechoslovak Chemical Communications (1959), 24, 3154-62
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA German
AB A series of derivs. of pyrimidine, 6-azauracil, hydantoin, guanidine, acetylurea, and quinazoline was tested for their inhibiting effect on the growth of Escherichia coli (% inhibition in the concentration 103, 102, and 10 γ per ml., resp., given). 4-Hydroxypyrimidine, 100, 62, 0; 2-thiocytosine,0,0,0. Uracil derivs.: 5-Et,0,0,0; 5-NO2, 100, 0, 0; 5-NH2 (I),0,0,0; yellow 5-diazo (II), 73, 9, 0; rose 5-diazo (III), 18, 0, 0; 5-cyano (IV), 16, 0, 0; 5-Br, 7, 0, 0; 5-iodo (V), 100,9,0; 5-MeNH,0,0,0; 5-AcNH,0,0,0; 6-Me (VI),0,0,0; 6-NH2(VII),0,0,0; 6-diazo (VIII),0,0,0; 2-thio, 92,0,0; 6-methyl-2-thio (IX),7,0,0; 6-amino-2-thio,0,0,0; 5-CONH2,0,0,0; 5-carbethoxy-6-nitro,0,0,0; 6-CH2CO2H, 0,0,0; 2-ethylthio-4-hydroxy-5-cyanopyrimidine, 67,10,0; 2-thioorotic acid, 10,0,0; 5-bromoorotic acid, 13,0,0. Dihydrouracil derivs.: 5-azido (X),9,0,0; 5-CNS,100,100,24; 5-Br (XI), 100, 32, 0; 5,5-dichloro-6-hydroxy (XII), 88, 4, 0; 5,5-dibromo-6-hydroxy (XIII) 100, 4, 0. Barbituric acid derivs.: 5-Et, 7, 0, 0; 5-Pr, 7, 0, 0; 5-iso-Pr, 7, 0, 0; 5,5-dibromo, 100, 100, 16. 6-Azauracil (XIV), 100, 100, 6. Derivs. of XIV: 5-Et,0,0,0; 5-iso-Pr,36,0,0; 5-tert-Bu,30, 14,0; 5-Am,100,25,0; 5-Ph,0,0,0; 5-CH2CO2Et, 21,0, 0; 2-thio,0,0,0; 2-thio-5-ethyl, 32,0,0; 2-thio-5-isopropyl,77, 0, 0; 2-thio-5-tert-butyl,0,0,0; 2-thio-5-amyl, 100,0,0; 2-thio-5-phenyl, 100, 57, 34; 2-carboxymethylthio-5-tert-butyl, 16,0,0; 2-carboxymethylthio-5-phenyl,0,0,0; 5-Br, 86,16,13. Dihydro-6-azauracil(XV),0,0,0. 6-Azathymine, 0,0,0. 2-Thio-6-azathymine,18,0,0. 5-Carbethoxymethylidenehydantoin, 49, 5, 0. Cyanoacetylguanidine, 9, 0, 0. RCONHCONH2 derivs. (R given): Me,0,0,0; CH2CN, 13, 3, 0; CH2N3(XVI),0,0,0; CH2Cl, 100,100,17; CHCl2,7,0, 0; CCl3,0,0,0; CH2Br (XVII),100,100,100(84% inhibition at a concentration of 1 γ per ml.); CBr3, 100,6,0; CH2I (XVIII), 100, 100 (95% inhibition at 0.5 γ per ml.). 4-Quinazolone, its 3-Ph, 3-PhCH2, and 2-HS derivs., 1-methyl-3-phenyl-1,2-dihydro-4-quinazolone, and 1-methyl-2-thioxo-3-phenyl-1,2-dihydro-4-quinazolone showed no inhibitory effect at concns. lower than 100 γ per ml. Halogen derivs. of acetylurea proved to be the most effective against E. coli. Similar results were obtained with Staphylococcus aureus and S. cerevisae. Since XVIII is a derivative of the known inhibitors, ICH2CO2H (XIX) and ICH2CONH2 (XX), the effect of these three compds. was compared. It was shown, that XVIII is two orders of magnitude more effective than XIX, and one order more than XX. New or modified prepns. are presented. Adding dropwise and with agitation at -15° 0.5 g. I in 2 ml. of 1:1 azeotropic HCl-H2O to 0.33 g. NaNO2 in 2 ml. H2O and crystallizing the yellow precipitate from H2O gave 0.5 g. II (the product did not melt, but explosively decomposed at 198°). A slow addition of 0.5 g. I in 2 ml. 1:3 azeotropic HCl-H2O to 0.33 g. NaNO2 in 2 ml. H2O at 0° with intense shaking gave a red precipitate, whose color finally changed to rose; crystallization from H2O yielded 0.55 g. III, decomposing explosively also at 198°. Refluxing 5.5 hrs. 0.5 g.

2-ethylthio-4-hydroxy-5-cyanopyrimidine, 25 ml. absolute EtOH, and 1.5 ml. concentrated H2SO4, concentrating the mixture in vacuo, and filtering off the precipitate gave 0.35 g. IV, m. 294° (decomposition) (EtOH). Mixing rapidly 3.32 g. KI in 4 ml. H2O with a filtered solution of 1.56 g. III, 8 ml. azeotropic HCl, and 6 ml. H2O, keeping the mixture until no gas was evolved (about 3 hrs.) filtering off the precipitate, washing with CHCl3, dissolving in hot H2O, filtering with C, decolorizing the filtrate with Na2S2O3 and cooling gave 0.5 g. V, m. 266-8° (H2O). Dissolving 112.5 g. IX (m. 320-3°) in a solution of 100 g. NaOH in 1500 ml. H2O, adding 150.5 g. ClCH2CO2H, boiling the mixture 30 min., cooling, acidifying with 275 ml. concentrated HCl, boiling further 90 min., and filtering with C gave 52.3 g. VI, m. 320° (H2O). Adding with agitation at 0° 3.3 g. NaNO2 in 20 ml. H2O to a suspension of 5 g. VII in 9 ml. concentrated HCl and 15 ml. H2O, keeping the mixture 30 min. at 0° with the addition of 10 ml. ice-H2O, separating the precipitate, and washing with ice-H2O gave 5 g. VIII, purple crystals. Boiling 4 hrs. 2 g. XI, 0.7 g. NaN3, and 100 ml. EtOH, evaporating the mixture in vacuo, and crystallizing the residue from H2O with C gave 0.6 g. X. XIII, decomposing partially at 220° (H2O), was prepared analogously to XII (Johnson, C.A. 37, 4737a). Hydrogenating 3.5 hrs. a suspension of 2.26 g. XIV in 20 ml. EtOH on 0.2 g. PtO2, adding hot H2O to dissolve the precipitate, filtering, and crystallizing gave XV, m. 210° (H2O). Refluxing 6.5 hrs. 0.2 g. XVII, 0.072 g. NaN3, and 10 ml. EtOH, evaporating in vacuo, and crystallizing the residue gave 0.05 g. XVI, m. 144-5° (decomposition) (H2O). 55 references.

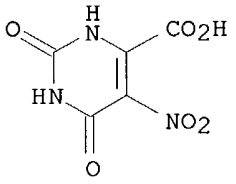
IT **100958-76-7**, 5-Pyrimidinecarboxylic acid, 2,4-dihydroxy-6-nitro-, ethyl ester
(bactericidal activity of)

RN 100958-76-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-nitro-2,4-dioxo-, ethyl ester (6CI) (CA INDEX NAME)



L6 ANSWER 138 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1958:25895 CAPLUS
DN 52:25895
OREF 52:4717h-i
TI Biochemical screening of pyrimidine antimetabolites. III. The testing of drugs against a system with a nonoxidative energy source
AU Stone, Joseph E.; Potter, Van R.
CS Univ. of Wisconsin, Madison
SO Cancer Research (1957), 17, 800-3
CODEN: CNREA8; ISSN: 0008-5472
DT Journal
LA Unavailable
AB Of 17 drugs which had demonstrated in vitro inhibitory activity against an oxidative system for conversion of orotic acid to the uridine nucleotides, 3 produced single or multiple blocking actions when retested against a nonoxidative system: these were 5-bromo-, 5-chloro-, and 5-fluoroorotic acids.
IT **17687-24-0**, Orotic acid, 5-nitro-
(effect on uracil nucleotide formation from orotic acid)
RN 17687-24-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



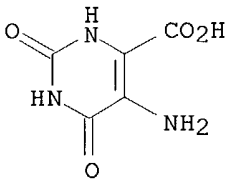
L6 ANSWER 139 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1952:23502 CAPLUS
DN 46:23502
OREF 46:4019i,4020a-i,4021a
TI Pyrimidinopyrimidines. I. Tetrahydroxyhomopurine and trihydroxyhomopurine, two "ring homologs" of uric acid and xanthine
AU Fischer, F. G.; Roch, J.
CS Univ. Wurzburg, Germany
SO Ann. (1951), 572, 217-29
DT Journal
LA Unavailable
AB So as to simplify the nomenclature of a new series of compds., F. and R. propose the term "homopurine" [instead of 7,9-pyrimidino-4',5',4,5-(1,3)-pyrimidine (C.A., pyrimido[5,4-d]pyrimidine)] for the parent substance (I). This entails the introduction of a C atom between positions 4 and 9 in the purine nucleus, and, strictly speaking, is not a homolog, although the relationship is obvious. (H2N)2CS (6 moles) in 500 cc. H2O stirred at 75-80° with 9 moles AcCH2CO2Et (II) and 9 moles dry powdered KOH, let stand 2 hrs., and treated with 2 l. H2O and 1.7-1.8 l. concentrated HCl (and small amts. of octanol) gave 800-810 g. SC.NH.CO.CH:CMe.NH (III) (also prepared in 75% yield by warming 6 moles (H2N)2CS with 7 moles II at 50-60° and introducing 7 moles KOH in 250 cc. H2O). To 50 cc. HNO3 (d. 1.48) and 20 cc. concentrated H2SO4 was added, very gradually, 14.2 g. III at 50-60°; when gas evolution ceased and the N-oxides had been removed, the mixture was heated 1 hr. on the steam bath and treated with 100 cc. H2O and 50 cc. 8 N KOH, giving 13-14 g. (crude) hydrated KO2CC:C(NO2).CO.NH.CO.NH (IV) [cf. Behrend, Ann. 240, 1(1887)]. IV (51.4 g.) was stirred into a solution of 115 g. tech. Na2S2O4 at 30°, the mixture acidified after 0.5 hr. with 130 cc. HCl, allowed to stand 3 hrs., and the resulting (30-31 g.) HO2CC:CNH2.CO.NH.CO.NH (V) purified through its NH4 salt (which, in excess NH4OH shows a brilliant (ultraviolet) violet-blue fluorescence, disappearing almost completely in aqueous KOH and giving a blue solution). Urea (120 g.) was stirred gradually into 34.2 g. finely powdered dry V at 135-40°, the temperature held 0.5 hr. at 140-50°, then raised to 210° (where it was kept a few min.), and the hot melt, sprinkled with H2O, freed from biuret, cyanuric acid, etc., by conversion into the di-Na salt (VI) of the 2,6,8,10-tetra-HO derivative (VII) of I (termed "hydroxyhomouric acid"), yielding VII on acidification with AcOH, and further purified by conversion into the NH4 salt, colorless needles. VII, microprisms, decompose (without m.) about 470°, is insol. in organic solvents, very difficultly soluble in H2O and aqueous acids, but quite soluble in concentrated H2SO4, from which it is precipitated unchanged by H2O. The alkali and NH4 salts are quite insol., but the piperidine, piperazine, and (HOCH2CH2)3N salts are relatively soluble The following salts of VII were prepared, and in some cases analyzed: VI (4H2O), long needles, di-K (? moles H2O); Pb, amorphous; Hg++, amorphous; Cu (C6H2O4N4Cu.H2O), bright green microcrysts.; Ni (C6H2O4N4Ni.H2O), greenish yellow (deeper yellow, when anhydrous); di-Ag (1H2O) (formed from VI and 2 moles AgNO3 in NH4OH), bright yellow flocks (olive-green, when dried); tri-Ag (C6HO4N4Ag3), formed when excess AgNO3 was used. VII (34.2 g.), 80 cc. HCONH2, and 10 cc. 95% HCO2H heated at 110-20°, followed by stepwise temperature increases up to 200°, and treatment of the melt with H2O, gave hydroxyhomoxanthine (VIII) (2,6,10-tri-HO derivative of I), purified through its mono-NH4 salt (3H2O), long needles. VIII retains 1 mole H2O tenaciously (and is rendered anhydrous only at 170° and 0.2 mm.), remaining unchanged up to 360°, decomposing without melting above this temperature, insol. in organic solvents, only slightly soluble in H2O, fails to reduce

AgNO3 in NH4OH or alkaline phosphomolybdate solns., is readily soluble in aqueous alkalies; di-Na salt (3H2O), long needles (titratable with aqueous HCl); mono-Na salt (from 1 equivalent 0.1 N NaOH; showing pH 8); di-K salt (very slightly soluble in H2O). The Ag and Pb salts of VIII (not analyzed) are amorphous. In the above synthesis of VIII, the 1st mother liquors contained 11-12 g. 5-formamidouracil (IX) (retaining 0.5 H2O at 130° and 0.2 mm.), m. 310° (decomposition) (from H2O), reducing aqueous phosphomolybdic acid, and hydrolyzed rapidly in alkaline solns. IX was also prepared by the formylation of aminouracil. Whereas various alkyl derivs. of VII and VIII are mentioned, descriptions of their syntheses are reserved for future publication.

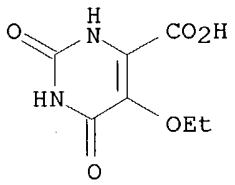
IT **7164-43-4**, Orotic acid, 5-amino-
(preparation of)

RN 7164-43-4 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



L6 ANSWER 140 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1929:16245 CAPLUS
DN 23:16245
OREF 23:1905b-e
TI Pyrimidines. CIV. Isouracil and its derivatives. Preliminary study of the methods of synthesis
AU Johnson, Treat B.; Caldwell, W. T.
CS Yale Univ.
SO Journal of the American Chemical Society (1929), 51, 873-80
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB cf. C. A. 20, 206. While the ultimate object of this work is the structure of orotic acid, which may be isouracilcarboxylic acid, the present paper is confined to the study of 2 different methods for synthesizing CO2H derivs. of isouracil; neither have led to practical results. CS(NH2)2 and EtOCH2. COCH(OEt)CO2Et are condensed by EtONa to 2-thio-4-ethoxymethyl-5-ethoxy-6-keto. pyrimidine, m. 178°, soluble in about 100 parts boiling H2O; heating with ClCH2CO2H gives 82% of the corresponding 2-keto derivative, m. 168°; heating with concentrated HCl at 120-40° for 2 h. removes the EtO groups, giving 93% of 2-keto-4-hydroxymelhyl-5-hydroxy-6-ketopyrimidine, yellow, does not m. 320°. With H2NC(SEt):NH there result 2-ethylmercapto-4-ethoxymethyl-5-ethoxy-6-ketopyrimidine, m. 123°; with PCl5 there is formed the 6-Cl derivative, light yellow oil, b9-10 165-6°, which is reduced by Zn in EtOH-H2O to 2-ethylmercapto-4-ethoxymethyl-5-ethoxypyrimidine, m. 167°; hydrolysis with HCl causes the evolution of EtSH, but the amount of material did not permit the continuation of the work. EtO2CCOCH(OEt)CO2Et and H2NC(SEt):NH condense to give a small amount of 2-ethylmercapto-4-carbethoxy-5-ethoxy-6-ketopyrimidine, m. 82-3°; the 2-keto derivative m. 230°, and 2-keto-4-carboxy-5-ethoxy-6-ketopyrimidine m. 260°; heating the latter at 1100 with concentrated HCl gives isobarbituric acid.
IT **14383-30-3**, Orotic acid, 5-ethoxy-
(preparation of)
RN 14383-30-3 CAPLUS
CN Orotic acid, 5-ethoxy- (8CI) (CA INDEX NAME)



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L2             STRUCTURE UPLOADED
L3             QUE L2 NOT L1
L4              11 S L3 SSS SAM
L5             346 S L3 SSS FUL

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L6             140 S L5

     FILE 'CAOLD' ENTERED AT 17:45:36 ON 20 MAY 2004

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L7              11 L5

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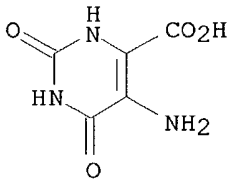
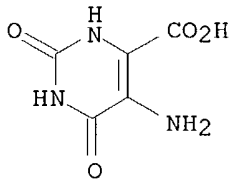
L7 ANSWER 1 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA64:2103h CAOLD
TI 5-aminoorotic acid
AU Goldner, Herbert; Trampau, L.
DT Patent

PATENT NO.	KIND	DATE
DE 39698		

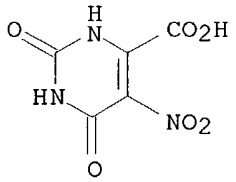
IT **7164-43-4**
RN 7164-43-4 CAOLD
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



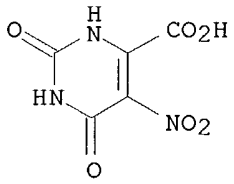
L7 ANSWER 2 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA59:13239f CAOLD
TI pattern of anticytogenic activity of pyrimidine derivs. on Neurospora crassa
AU Rauen, Hermann M.; Nonhoff, R.
IT **7164-43-4 17687-24-0**
RN 7164-43-4 CAOLD
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



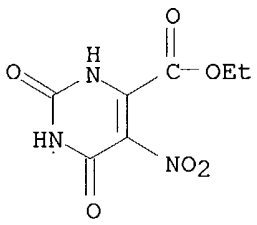
RN 17687-24-0 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



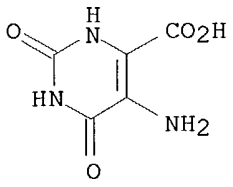
L7 ANSWER 3 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA58:12151f CAOLD
TI metal complexation with pyrimidine derivs. - (II) spectrophotometric studies
AU Tucci, Edmond R.; Li, N. C.
IT **17687-24-0**
RN 17687-24-0 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



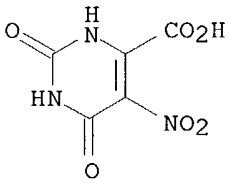
L7 ANSWER 4 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA57:7002d CAOLD
TI electrochem. characteristics of organic compds. - (IX) pyrimidine compds.
AU Glicksman, Richard
IT **52047-16-2**
RN 52047-16-2 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



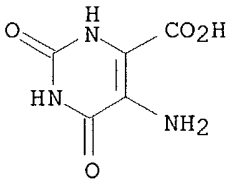
L7 ANSWER 5 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA57:6307e CAOLD
TI properties of triphosphopyridine nucleotide-linked dihydroorotic dehydrogenase
AU Udaka, Shigezo; Vennesland, B.
IT **7164-43-4**
RN 7164-43-4 CAOLD
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



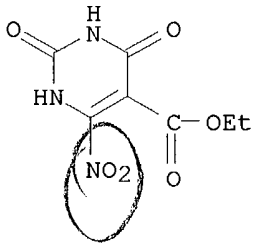
L7 ANSWER 6 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA56:2035g CAOLD
TI acid dissociation consts. and complex formation consts. of several pyrimidine derivs.
AU Tucci, Edmond R.; Doody, (Brother Edward); Li, N. C.
IT **17687-24-0**
RN 17687-24-0 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



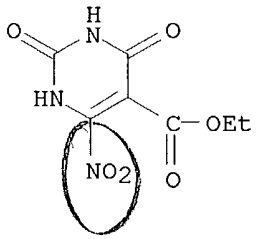
L7 ANSWER 7 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA55:6603e CAOLD
TI isolation of deoxyribonucleic acid from bacterial exts. by precipitation with streptomycin
AU Cohen, Seymour S.; Lichtenstein, J.
IT **7164-43-4**
RN 7164-43-4 CAOLD
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



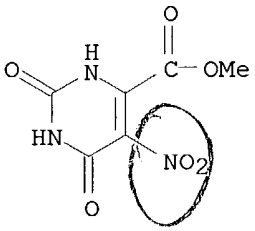
L7 ANSWER 8 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA55:4861f CAOLD
TI pyrimidine derivs. as new types of plant stimulants
AU Sormova, Z.; Melichar, O.; Sorm, F.
IT **100958-76-7**
RN 100958-76-7 CAOLD
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-nitro-2,4-dioxo-, ethyl ester (6CI) (CA INDEX NAME)



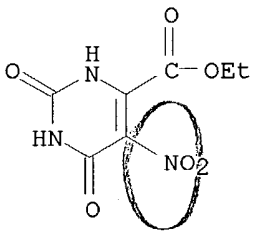
L7 ANSWER 9 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA54:4611a CAOLD
TI nucleic acid components and their analogs - (III) antimicrobial effect of pyrimidine analogs and related compds.
AU Gut, Jiri; Moravek, J.; Parkanyi, C.; Prystas, M.; Skoda, J.; Sorm, F.
IT **100958-76-7**
RN 100958-76-7 CAOLD
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-nitro-2,4-dioxo-, ethyl ester (6CI) (CA INDEX NAME)



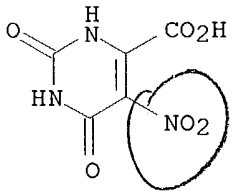
L7 ANSWER 10 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA52:20183d CAOLD
TI glyoxalinopyrimidines - (II)
AU Clark, Jim; Ramage, G. R.
IT **6311-73-5 52047-16-2**
RN 6311-73-5 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



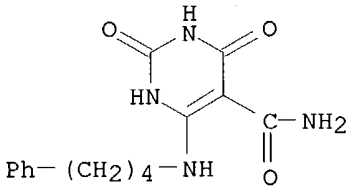
RN 52047-16-2 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



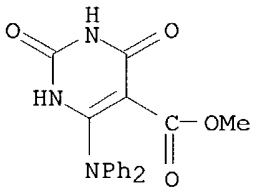
L7 ANSWER 11 OF 11 CAOLD COPYRIGHT 2004 ACS on STN
AN CA52:4717i CAOLD
TI enzymic hydrolysis of imidazoleacryloylcholine and imidazolepropionylcholine by cholinesterases
AU Grelis, Mary E.; Tabachnick, I. I. A.
IT **17687-24-0**
RN 17687-24-0 CAOLD
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-nitro-2,6-dioxo- (9CI) (CA INDEX NAME)



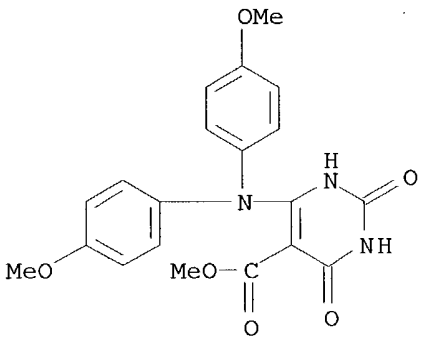
L6 ANSWER 75 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:422414 CAPLUS
DN 99:22414
TI Chemistry of 5-pyrimidinecarboxaldehydes
AU Bell, Lawrence; McGuire, H. Michael; Freeman, G. Andrew
CS Dep. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA
SO Journal of Heterocyclic Chemistry (1983), 20(1), 41-4
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 99:22414
AB Selective hydrolysis of 2-amino-4,6-dichloro-5-pyrimidinecarboxaldehyde, (I) gave 2-amino-4-chloro-1,6-dihydro-6-oxo-5-pyrimidinecarboxaldehyde. The oxime of I rearranged to 2-amino-4-chloro-1,6-dihydro-6-oxo-5-pyrimidinecarbonitrile (II). Reaction of II with 4-phenylbutylamine resulted in the displacement of the 4-chloro atom to give compound III (R = CN, R1 = H) (IV). Hydrolysis of the cyano function of IV gave amides III (R = CONH2, R1 = SO3H; R = CONH2, R1 = H) and V depending on reaction conditions. A discussion of the 1H-NMR spectrum of 2-amino-1,6-dihydro-6-oxo-4-[(4-phenylbutyl)amino]-5-pyrimidinecarboxaldehyde is presented.
IT **85840-29-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85840-29-5 CAPLUS
CN 5-Pyrimidinecarboxamide, 1,2,3,4-tetrahydro-2,4-dioxo-6-[(4-phenylbutyl)amino]- (9CI) (CA INDEX NAME)



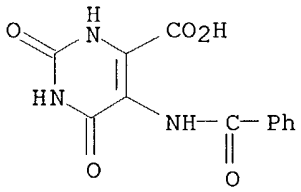
L6 ANSWER 45 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:583231 CAPLUS
DN 115:183231
TI Synthesis of pyrimidine derivatives using N-bis(methylthio)methylenecyanamide
AU Tominaga, Yoshinori; Ohno, Syuichirou; Kohra, Shinya; Fujito, Hiroshi; Mazume, Hisako
CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, 852, Japan
SO Journal of Heterocyclic Chemistry (1991), 28(4), 1039-42
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 115:183231
AB (MeS)2C:NCN reacted with active methylene compds. (Me cyanoacetate, di-Me malonate, Et acetoacetate, Et phenylacetate) in the presence of K2CO3 or KOH in DMSO followed by the treatment using an appropriate base or acid to give the corresponding 6-methylthiouracil derivs. I (R = SMe, R1= cyano, CO2Me, COMe, Ph) in 15-80% yields. These uracil derivs. are useful intermediates for the synthesis of 6-aminouracils and fused pyrimidine derivs. Thus, the reactions of I (R = SMe, R1 = cyano) with H2NXH (X = O, NH, NPh) gave isoxazolopyrimidine II (X = O) and pyrazolopyrimidines II (X = NH, NPh) resp. R2NH2 (R2 = Ph, substituted Ph, PhCH2) reacted with I (R = SMe, R1 = cyano) to give I (R = NHR2).
IT **136411-49-9P 136411-50-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 136411-49-9 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 6-(diphenylamino)-1,2,3,4-tetrahydro-2,4-dioxo-, methyl ester (9CI) (CA INDEX NAME)



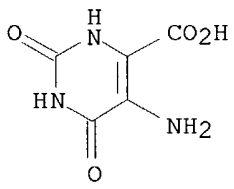
RN 136411-50-2 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 6-[bis(4-methoxyphenyl)amino]-1,2,3,4-tetrahydro-2,4-dioxo-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 79 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:484779 CAPLUS
DN 97:84779
TI Synthesis and biological properties of some 5-aminoorotic acid derivatives
AU Machon, Zdzislaw; Jasztold-Howorko, Ryszard
CS Inst. Chem. Phys., Med. Acad., Wroclaw, 50-137, Pol.
SO Polish Journal of Pharmacology and Pharmacy (1981), 33(5), 545-52
CODEN: PJPPAA; ISSN: 0301-0244
DT Journal
LA English
AB 2,4-Dihydroxy-5-benzoylaminopyrimidine-6-carboxylic acid in the reaction with SOCl2 gave 1-benzoyl-2-oxo-4,6-dihydroxyazetino[3,2-d]pyrimidine which reacted with aliphatic and aromatic amines in EtOH to give I (R = COPh or COC6H5-Cl-p; R1 = NH2; NHPh, OEt, etc.) and ethyl 2,4-dihydroxy-5-benzoylaminopyrimidine-6-carboxylate. Some I were centrally active and showed antiinflammatory and analgesic activity.
IT **59662-86-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 59662-86-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

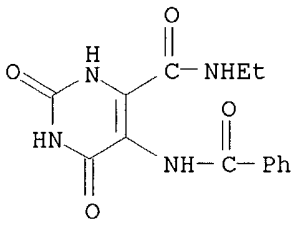


IT **7164-43-4DP**, derivs. **82241-25-6P 82241-26-7P**
82241-27-8P 82241-29-0P 82241-30-3P
82241-32-5P 82241-33-6P 82241-34-7P
82241-35-8P 82241-36-9P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

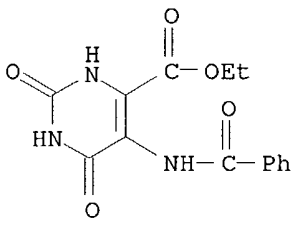


RN 82241-25-6 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-ethyl-1,2,3,6-tetrahydro-2,6-

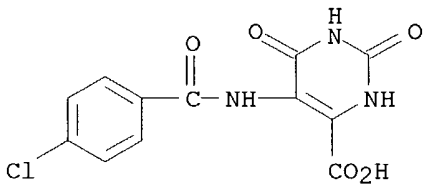
dioxo- (9CI) (CA INDEX NAME)



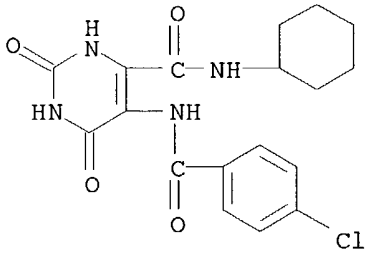
RN 82241-26-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



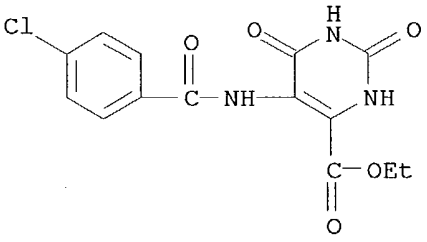
RN 82241-27-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorobenzoyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



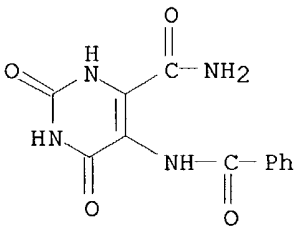
RN 82241-29-0 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-[(4-chlorobenzoyl)amino]-N-cyclohexyl-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



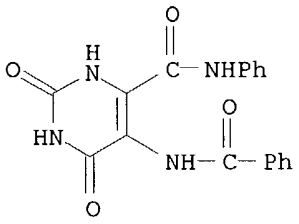
RN 82241-30-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorobenzoyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



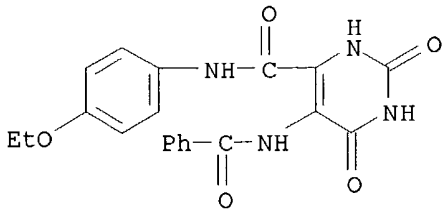
RN 82241-32-5 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



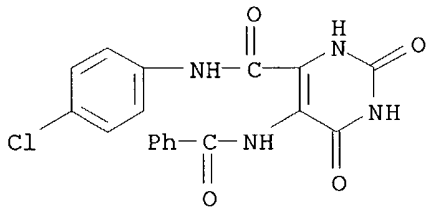
RN 82241-33-6 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo-N-phenyl- (9CI) (CA INDEX NAME)



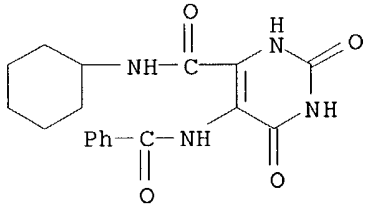
RN 82241-34-7 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(4-ethoxyphenyl)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 82241-35-8 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(4-chlorophenyl)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



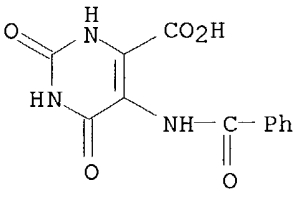
RN 82241-36-9 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-cyclohexyl-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



IT **82241-31-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82241-31-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(benzoylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, compd. with N-ethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 59662-86-1
CMF C12 H9 N3 O5



CM 2

CRN 109-89-7
CMF C4 H11 N

L6 ANSWER 37 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:630786 CAPLUS
DN 121:230786
TI (Phenylsulfonamido)pyrimidine endothelin receptor inhibitors
IN Breu, Volker; Burri, Kaspar; Cassal, Jean Marie; Clozel, Martine; Hirth, Georges; Loeffler, Bernd Michael; Mueller, Marcel; Neidhart, Werner; Ramuz, Henri
PA F. Hoffmann-La Roche AG, Switz.
SO Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

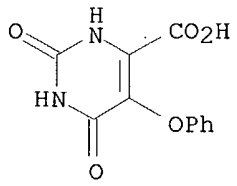
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 601386	A1	19940615	EP 1993-118869	19931124
	EP 601386	B1	20030205		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	AT 232204	E	20030215	AT 1993-118869	19931124
	ES 2190430	T3	20030801	ES 1993-118869	19931124
	ZA 9309091	A	19940610	ZA 1993-9091	19931203
	AU 9352189	A1	19940623	AU 1993-52189	19931206
	AU 669019	B2	19960523		
	HU 65689	A2	19940728	HU 1993-3458	19931206
	IL 107884	A1	19980310	IL 1993-107884	19931206
	RU 2156241	C2	20000920	RU 1993-54179	19931207
	CA 2110944	AA	19940611	CA 1993-2110944	19931208
	BR 9304980	A	19940614	BR 1993-4980	19931208
	US 5420129	A	19950530	US 1993-164167	19931208
	CZ 288030	B6	20010411	CZ 1993-2684	19931208
	NO 9304502	A	19940613	NO 1993-4502	19931209
	JP 06211810	A2	19940802	JP 1993-309219	19931209
	JP 08026006	B4	19960313		
	CN 1095375	A	19941123	CN 1993-120171	19931209
	CN 1049430	B	20000216		
	PL 178329	B1	20000428	PL 1993-301394	19931209
	FI 9305555	A	19940611	FI 1993-5555	19931210
PRAI	CH 1992-3777	A	19921210		
	CH 1992-3799	A	19921211		
	CH 1993-3114	A	19931014		

OS MARPAT 121:230786
AB The title compds. [I; R1 = H, lower alkyl, lower alkoxy, lower alkylthio, halogen, trifluromethyl; R2 = H, lower alkyl, haloegn, lower alkoxy, trifluoromethyl, etc.; R3 = H, lower alkyl, halogen, lower alkylthio, trifluromethyl, trifluoromethoxy, lower alkoxy; R4 = H, lower alkyl, trifluoromethyl, lower alkoxy, lower alkylthio, hydroxyalkyl, lower alkylfulfinyl, etc.; R5, R8 = H, halogen, trifluoromethyl, lower alkoxy lower alkylthio, CN; R2R3, R5R6, R6R7 may form a butadienyl, methylene dioxy, ethylene dioxy, or isopropylidienedioxy bridging group; X = O, S; Y = CHO, (un)substituted alkyl, etc.; n = 0, 1], which are endothelin receptor inhibitors useful for the treatment of hypertension, ischemia (no data), etc., are prepared and I-containing formulations presented. Thus, 4-tert-butyl-N-[5-(2-chloro-5-methoxyphenoxy)-6-(2-hydroxyethoxymethyl)-2-(morpholin-4-yl)pyrimidin-4-yl]benzenesulfonimide, m.p. 162-164°, was prepared and demonstrated IC50 against the binding of 125I-endothelin of 0.035 μM.
IT **14383-34-7 157415-44-6**
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of (phenylsulfonamido)pyrimidine endothelin receptor inhibitors)

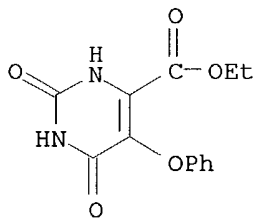
RN 14383-34-7 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-phenoxy- (9CI) (CA INDEX NAME)

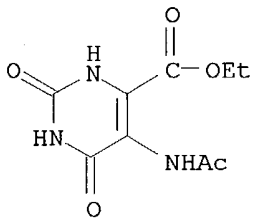


RN 157415-44-6 CAPLUS

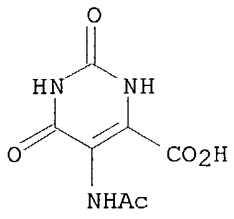
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 25 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:98933 CAPLUS
DN 126:171552
TI Synthesis of new 5-aminoorotic acid derivatives as antimicrobial agents
AU El Kolli, Meriem; Mahamoud, Abdallah; Coulibaly, Adama; Chevalier, Jacqueline; Cremieux, Andre; Barbe, Jacques
CS Fac. pharmacie, GERCTOP-URA CNRS 1411, Marseille, 13385, Fr.
SO Heterocyclic Communications (1996), 2(6), 531-537
CODEN: HCOMEX; ISSN: 0793-0283
PB Freund
DT Journal
LA English
AB Reaction between 5-aminoorotic acid and alkyl halides in DMF gave esters and/or 1-alkyl substituted orotates I (R = Me, Et, n-Pr, n-pentyl, piperidino, n-hexyl, R1 = R2 = H; R = R1 = n-Pr, n-pentyl, R2 = H) depending upon exptl. conditions. These compds. were converted into the corresponding 5-acylamino derivs. The latter derivs. were tested in vitro against gram pos. and gram neg. bacteria. The great majority of them show significant growth inhibitory effects. Moreover, some others are specific inhibitors for gram pos. bacteria.
IT **40598-10-5P 187232-27-5P 187232-28-6P**
187232-29-7P 187232-35-5P 187232-38-8P
187232-39-9P 187232-40-2P 187232-41-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of aminoorotic acid derivs.)
RN 40598-10-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)

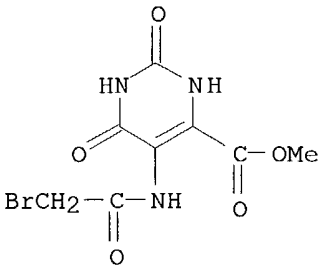


RN 187232-27-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)

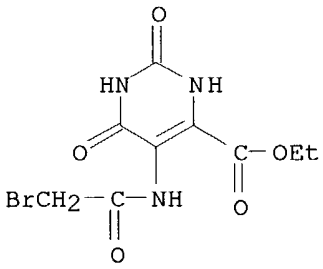


RN 187232-28-6 CAPLUS

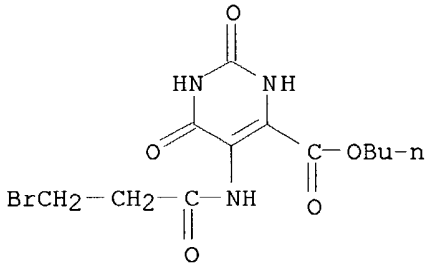
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



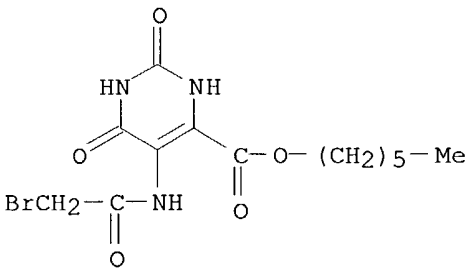
RN 187232-29-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



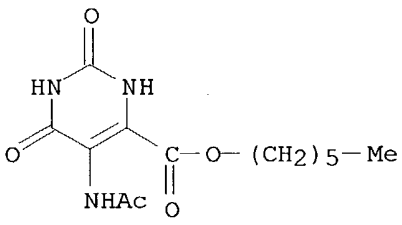
RN 187232-35-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



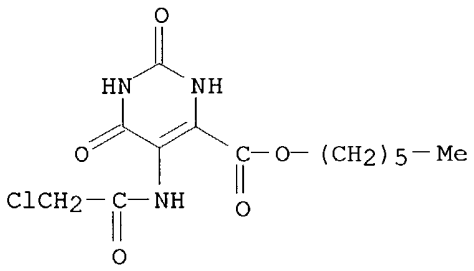
RN 187232-38-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



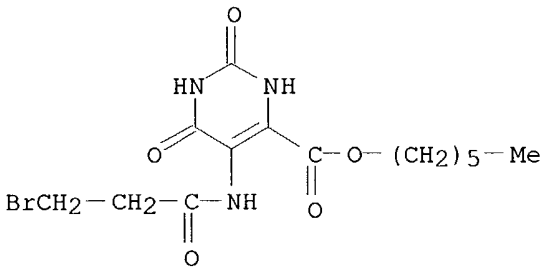
RN 187232-39-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



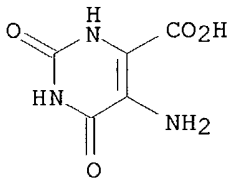
RN 187232-40-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



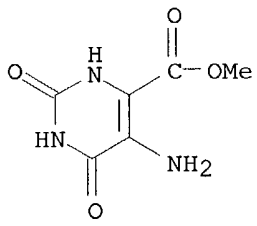
RN 187232-41-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



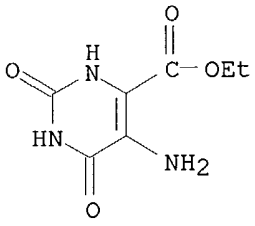
IT **7164-43-4,** 5-Aminoorotic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and bactericidal activity of aminoorotic acid derivs.)
RN 7164-43-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



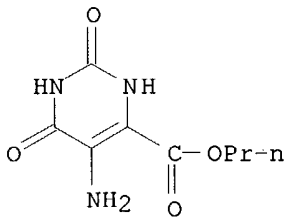
IT **19796-65-7P 40598-01-4P 187232-21-9P**
187232-22-0P 187232-23-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bactericidal activity of aminoorotic acid derivs.)
RN 19796-65-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



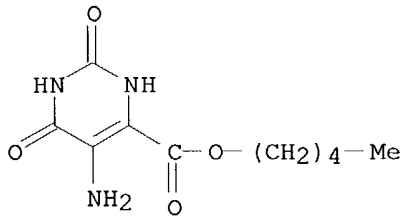
RN 40598-01-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



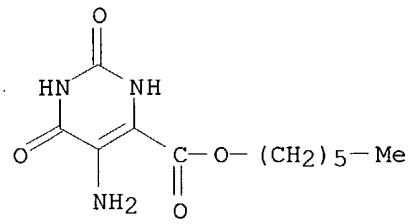
RN 187232-21-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, propyl ester (9CI) (CA INDEX NAME)



RN 187232-22-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, pentyl ester (9CI) (CA INDEX NAME)



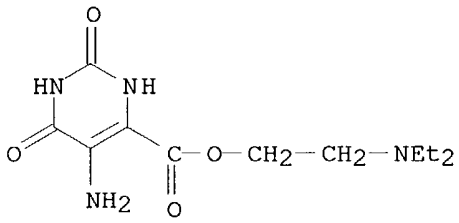
RN 187232-23-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, hexyl ester (9CI) (CA INDEX NAME)



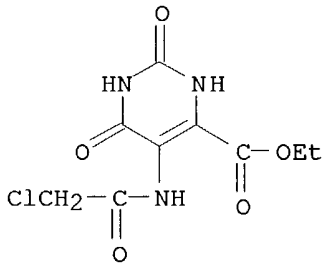
IT **187232-24-2P 187232-30-0P 187232-31-1P 187232-32-2P 187232-33-3P 187232-34-4P**

187232-36-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and bactericidal activity of aminoorotic acid derivs.)

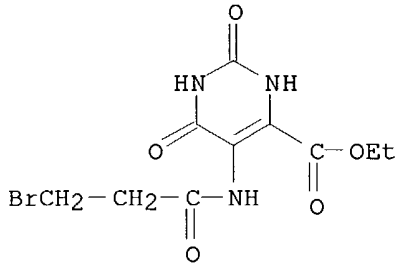
RN 187232-24-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, 2-(diethylamino)ethyl ester (9CI) (CA INDEX NAME)



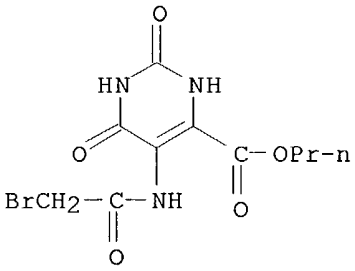
RN 187232-30-0 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



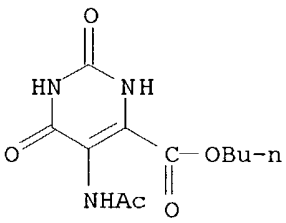
RN 187232-31-1 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(3-bromo-1-oxopropyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



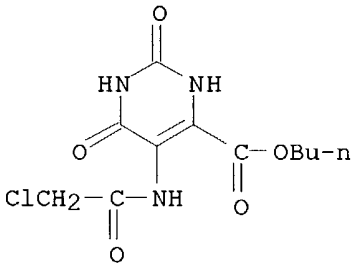
RN 187232-32-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, propyl ester (9CI) (CA INDEX NAME)



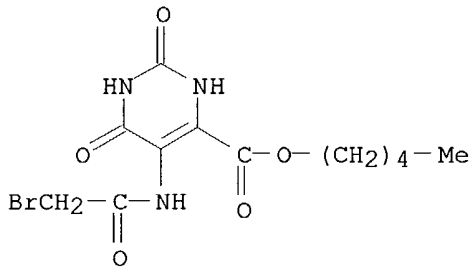
RN 187232-33-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



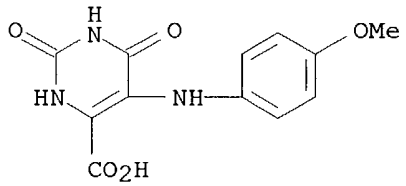
RN 187232-34-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(chloroacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, butyl ester (9CI) (CA INDEX NAME)



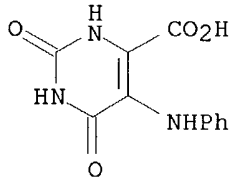
RN 187232-36-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(bromoacetyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo-, pentyl ester (9CI) (CA INDEX NAME)



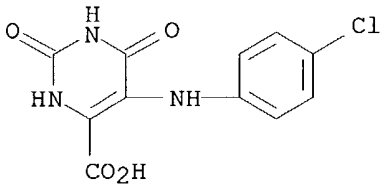
L6 ANSWER 106 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:136212 CAPLUS
DN 78:136212
TI Synthesis of 5-phenylamino derivatives of orotic acid
AU Britikova, N. E.; Belova, L. A.; Chkhikvdze, K. A.; Magidson, O. Yu.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1973), (2), 273-5
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
AB The title compds. (I; R = MeO, H, Cl, MeO2C, R1 = H; R = R1 = O2N; R2 = R3 = H) were prepared in 15-64% yields by amination of 5-bromooroctic acid with the appropriate amine in HOCH2CH2OH at .apprx.150°. Methylation of I(R = MeO, R1-R3 = H) with (MeO)2SO2 in aqueous alc. containing KOH at 12-15° for 1 hr gave 35% anisidinoorotic acid I (R = MeO, R2 = H, R2 = R3 = Me); similar methylation at 3-5° for 20 min yielded 37% I (R = OMe, R1 = R3 = H, R2 = Me).
IT **6964-60-9P 40598-17-2P 40598-18-3P**
40598-19-4P 40598-20-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 6964-60-9 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[(4-methoxyphenyl)amino]-2,6-dioxo- (9CI) (CA INDEX NAME)



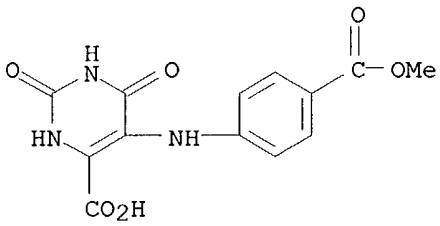
RN 40598-17-2 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-5-(phenylamino)-(9CI) (CA INDEX NAME)



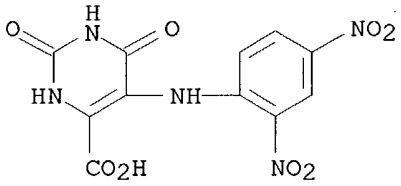
RN 40598-18-3 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(4-chlorophenyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



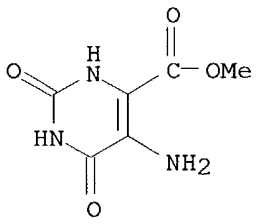
RN 40598-19-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-5-[[4-(methoxycarbonyl)phenyl]amino]-2,6-dioxo- (9CI) (CA INDEX NAME)



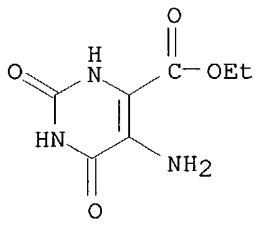
RN 40598-20-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-[(2,4-dinitrophenyl)amino]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



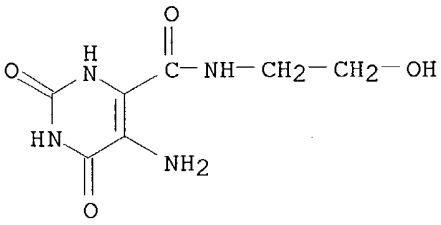
L6 ANSWER 105 OF 140 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:136214 CAPLUS
DN 78:136214
TI 5-Aminoorotic acid derivatives
AU Britikova, N. E.; Belova, L. A.; Chkhikvadze, K. A.; Magidson, O. Yu.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1973), (2), 270-2
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
AB Pyrimidooxazine I was obtained in 91% yield by cyclization of 5-aminoorotic acid with Ac2O. Cleavage of I with RONa in ROH gave .apprx.60% yield of acetyl derives. II (R = OEt, OMe, R1 = Ac), which were readily deacetylated by HCl to give 48-54% II (R = OEt, OMe, R1 = H). Heating the latter with the appropriate amine gave 65% and 77% of orotamides II (R = PhCH2NH, HOCH2CHwNH, R1 = H). Treatment of I with RNH2 gave 36-83% II (R = H2NNH, H2N, PhNH, Et2NCH2CH2NH, R1 = Ac).
IT **19796-65-7P 40598-01-4P 40598-03-6P**
40598-04-7P 40598-05-8P 40598-06-9P
40598-07-0P 40598-08-1P 40598-10-5P
40598-11-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19796-65-7 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



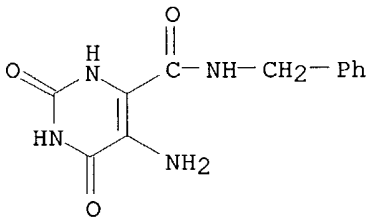
RN 40598-01-4 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



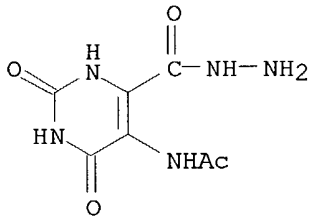
RN 40598-03-6 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-amino-1,2,3,6-tetrahydro-N-(2-hydroxyethyl)-2,6-dioxo- (9CI) (CA INDEX NAME)



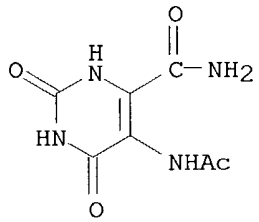
RN 40598-04-7 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



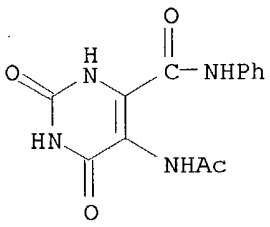
RN 40598-05-8 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, hydrazide (9CI) (CA INDEX NAME)



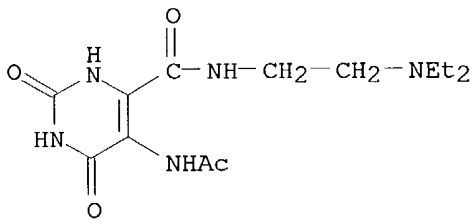
RN 40598-06-9 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



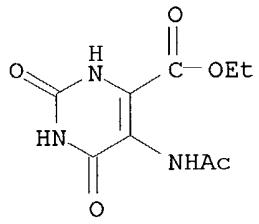
RN 40598-07-0 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-N-phenyl- (9CI) (CA INDEX NAME)



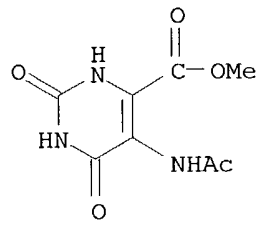
RN 40598-08-1 CAPLUS
CN 4-Pyrimidinecarboxamide, 5-(acetylamino)-N-[2-(diethylamino)ethyl]-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



RN 40598-10-5 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 40598-11-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-(acetylamino)-1,2,3,6-tetrahydro-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)

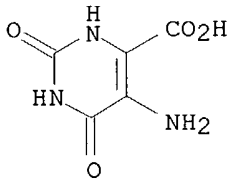


IT **7164-43-4**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetic anhydride)

RN 7164-43-4 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 5-amino-1,2,3,6-tetrahydro-2,6-dioxo- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              30.45     857.52

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00     -97.02

STN INTERNATIONAL LOGOFF AT 17:46:07 ON 20 MAY 2004
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